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STRUCTURE FILE UPDATES: 30 NOV 2009 HIGHEST RN 1194522-11-6
DICTIONARY FILE UPDATES: 30 NOV 2009 HIGHEST RN 1194522-11-6
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New CAS Information Use Policies, enter HELP USAGETERMS for details.

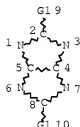
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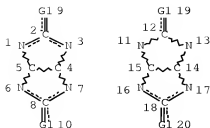
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STEREO ATTRIBUTES: NONE
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FILE COVERS 1907 - 2 Dec 2009 VOL 151 ISS 23
 FILE LAST UPDATED: 1 Dec 2009 (20091201/ED)
 REVISED CLASS FIELDS (/NCL) LAST RELOADED: Aug 2009
 USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Aug 2009

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d 144 bib abs hitstr tot

L44 ANSWER 1 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN

AN 2005:1056334 HCAPLUS Full-text

DN 144:311666

TI Host-guest complexes of cucurbit[8]uril with phenanthrolines and some methyl derivatives

AU Fu, Haiyan; Xue, Saifeng; Mu, Lan; Du, Ying; Zhu, Qianjiang; Tao, Zhu; Zhang, Jianxin; Day, Anthony I.

CS Institute of Applied Chemistry, Guizhou University, Guiyang, 550025, Peop. Rep. China

SO Science in China, Series B: Chemistry (2005), 48(4), 305-314

CODEN: SCBCFQ; ISSN: 1006-9291

PB Science in China Press

DT Journal

LA English

AB The host-guest relationship between cucurbit[8]uril, phenanthrolines and some Me substituted 1,10-phenanthrolines has been investigated by using 1H NMR spectroscopy and fluorescence spectroscopy. The results showed that phenanthrolines as mol. guests bind in the cavity and portal of cucurbit[8]uril in a ratio of 2:1 (guest to host). The phenanthroline isomers 1,10-, 1,7- and 4,7- showed red shifts between 47 and 108 nm and pronounced increases in fluorescence intensity. These same isomers produced inclusion complexes with cucurbit[8]uril which had moderate to fast exchange rates on the 1H NMR time scale. The Me substituted 1,10-phenanthrolines studied gave stable inclusion complexes in a ratio of 2:1 which showed slow exchange rates. These guests formed π - π stacked pairs which were cavity bound but also partly protruded from only one portal forming unsym. host-guest complexes. In addition, these π - π stacked pairs formed orientation isomers within the confines of the cucurbit[8]uril cavity.

IT 879547-41-8 879547-45-2 879547-48-5

879547-51-0 879547-54-3 879547-59-8

RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative) (inclusion complex; host-guest complexes of cucurbit[8]uril with phenanthrolines and some Me derivs.)

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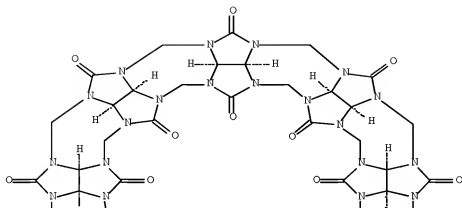
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CRN 259886-51-6

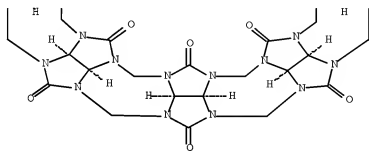
CMF C48 H48 N32 O16

Relative stereochemistry.

PAGE 1-A



PAGE 2-A



CM 2

CRN 3829-86-5

CMF C12 H8 N2 . C1 H



● HCl

RN 879547-45-2 HCAPLUS

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(CA INDEX NAME)

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CRN 879547-43-0

CMF C12 H8 N2 . Cl H



● HCl

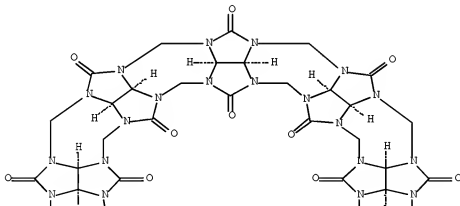
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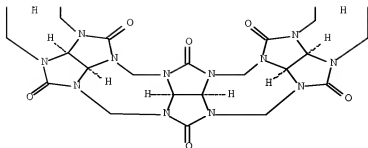
CMF C48 H48 N32 O16

Relative stereochemistry.

PAGE 1-A



PAGE 2-A



RN 879547-48-5 HCAPLUS
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 g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
 1,4,6,8,10,12,14,16,18,21,23,25,27,29,31,33-hexadecone, hexadecahydro-,
 stereoisomer, compd. with 2,9-dimethyl-1,10-phenanthroline
 monohydrochloride (1:2) (9CI) (CA INDEX NAME)

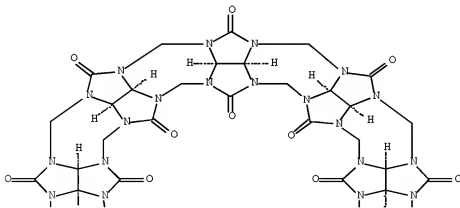
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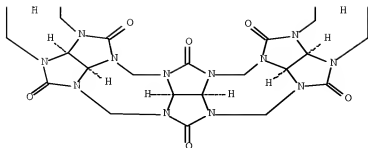
CMF C48 H48 N32 O16

Relative stereochemistry.

PAGE 1-A



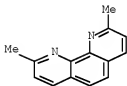
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CM 2

CRN 7296-20-0

CMF C14 H12 N2 . Cl H



● HCl

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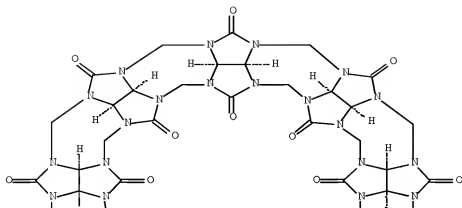
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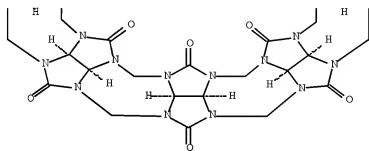
CMF C48 H48 N32 O16

Relative stereochemistry.

PAGE 1-A



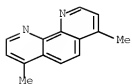
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CM 2

CRN 23484-50-6

CMF C14 H12 N2 . Cl H



● HCl

RN 879547-54-3 HCAPLUS

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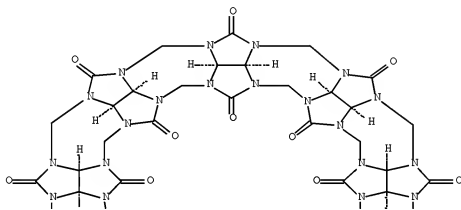
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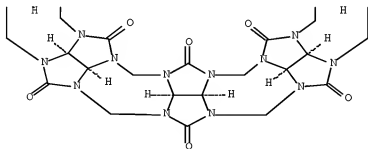
CMF C48 H48 N32 O16

Relative stereochemistry.

PAGE 1-A



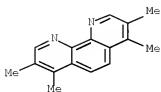
PAGE 2-A



CM 2

CRN 37386-28-0

CMF C16 H16 N2 . Cl H



● HCl

RN 879547-59-8 HCAPLUS
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 '':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-
 g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
 1,4,6,8,10,12,14,16,18,21,23,25,27,29,31,33-hexadecone, hexadecahydro-,
 stereoisomer, compd. with 1,7-phenanthroline monohydrochloride (1:2) (9CI)
 (CA INDEX NAME)

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CRN 879547-56-5

CMF C12 H8 N2 . C1 H



● HCl

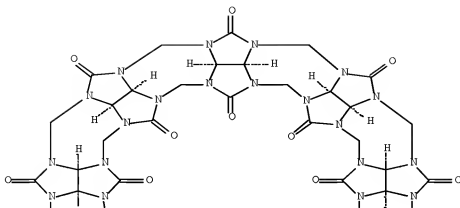
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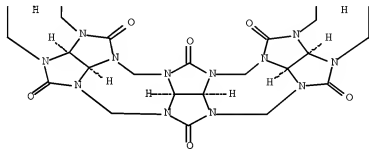
CMF C48 H48 N32 O16

Relative stereochemistry.

PAGE 1-A



PAGE 2-A



OSC.G 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD (8 CITINGS)
 RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 2 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN

AN 2005:1042246 HCAPLUS [Full-text](#)

DN 143:347171

TI Method for preparing compounds comprising cucurbituril groups

IN Day, Anthony Ivan

PA Unisearch Limited, Australia

SO PCT Int. Appl., 56 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

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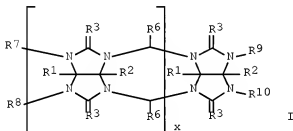
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PRAI AU 2004-901473 A 20040319 <--
 WO 2005-AU396 W 20050318 <--

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OS CASREACT 143:347171; MARPAT 143:347171

GI



AB The present invention provides a method for preparing compds. comprising a plurality of cucurbituril groups. The method comprises forming a mixture comprising one or more compds. of the formula A-L-A wherein L is a linking group and A is group of the formula I [R1 and R2 independently = bond with L or univalent radical, or R1,R2 and the carbon atoms to which they are bound together from an (un)substituted cyclic group, or R1 of one unit and R2 of adjacent unit from a bond or divalent radical, etc.; R3 = O, S, NH, etc.; R6 = bond with L, H, alkyl, and aryl; R7 and R8 or R9 and R10 independently = H and CHR6OR6, or R7 and R8 together form the group -CHR6OCHR6-; x = 0-10 with provisions], and an acid, and exposing the mixture to conditions effective for at least some of the groups A to form cucurbituril groups.

IT 80262-44-8E, Cucurbituril, derivs.

RL: PNU (Preparation, unclassified)

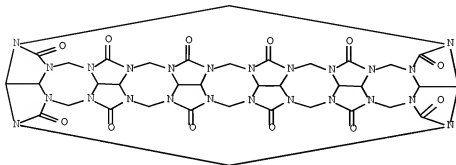
(preparation of dimer, trimer and tetramers of glycolurils useful for preparing

compound containing plurality of cucurbituril groups)

RN 80262-44-8 HCAPLUS

CN 1H, 4H, 14H, 17H-2, 16:3, 15-Dimethano-
 5H, 6H, 7H, 8H, 9H, 10H, 11H, 12H, 13H, 18H, 19H, 20H, 21H, 22H, 23H, 24H, 25H, 26H-

2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24a,25a,26a-tetracosazabispentaleno[1''',6'''':5'',6'',7''']cycloocta[1'',2'',3''':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,17,19,21,23,25-dodecone, dodecahydro- (CA INDEX NAME)



IT 848440-50-6 865813-88-3 865813-93-0

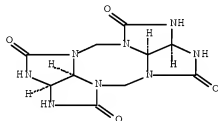
RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of dimer, trimer and tetramers of glycolurils useful for preparing compound containing plurality of cucurbituril groups)

RN 848440-50-6 HCAPLUS

CN 5H,10H-2,3,4a,5a,7,8,9a,10a-Octaazacycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,9(2H,3H,7H,8H)-tetrone, tetrahydro-, stereoisomer (CA INDEX NAME)

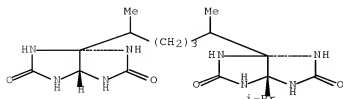
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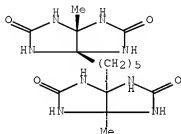
CN Imidazo[4,5-d]imidazole-2,5(1H,3H)-dione, 3a-[5-(cis-hexahydro-2,5-dioxoimidazo[4,5-d]imidazol-3a(1H)-yl)-1-methylhexyl]tetrahydro-6a-(1-methylethyl)-, cis- (CA INDEX NAME)

Relative stereochemistry.



RN 865813-93-0 HCAPLUS
 CN Imidazo[4,5-d]imidazole-2,5(1H,3H)-dione,
 3a,3'a-(1,5-pentenediyl)bis[tetrahydro-6a-methyl-, (cis,cis)- (9CI) (CA
 INDEX NAME)

Relative stereochemistry.



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 865813-94-1P

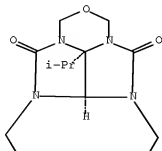
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of dimer, trimer and tetramers of glycolurils useful for
 preparing compound containing plurality of cucurbituril groups)

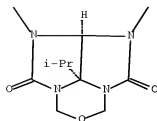
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 CN 1H,3H,4H,5H,6H,7H,9H,10H,11H,12H-2,8-Dioxa-3a,4a,5a,6a,9a,10a,11a,12a-
 octaazadibenzo[gh,g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-4,6,10,12-
 tetrone, tetrahydro-10c,12b-bis(1-methylethyl)-, stereoisomer (9CI) (CA
 INDEX NAME)

Relative stereochemistry.

PAGE 1-A



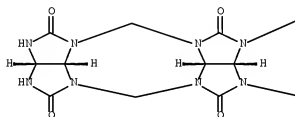
PAGE 2-A



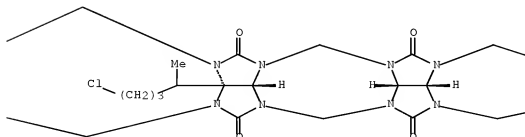
RN 848440-51-7 HCAPLUS
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 2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 13, 14, 15a, 16a, 17a, 18a, 19a, 20a, 21a, 22a-
 Eicosaazabispentaleno[1'', 6'':5'', 6'', 7'']cycloocta[1'', 2'', 3'':3', 4']pe
 ntaleno[1', 6':5, 6, 7]cycloocta[1, 2, 3-cd:1', 2', 3'-gh]pentalene-
 1, 4, 6, 8, 10, 12, 15, 17, 19, 21 (2H, 3H, 13H, 14H)-decone,
 19b-(4-chloro-1-methylbutyl)decahydro-, stereoisomer (9CI) (CA INDEX
 NAME)

Relative stereochemistry.

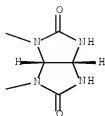
PAGE 1-A



PAGE 1-B



PAGE 1-C

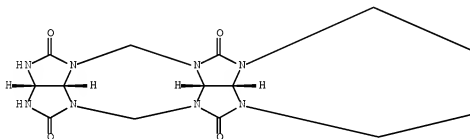


RN 848440-52-8 HCAPLUS

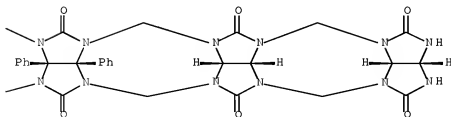
CN 5H, 6H, 7H, 8H, 9H, 10H, 11H, 16H, 17H, 18H, 19H, 20H, 21H, 22H-
2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 13, 14, 15a, 16a, 17a, 18a, 19a, 20a, 21a, 22a-
Eicosazabispentaleno[1''', 6''': 5'', 6'', 7'']cycloocta[1'', 2'', 3'': 3', 4']pe
ntaleno[1', 6': 5, 6, 7]cycloocta[1, 2, 3-cd: 1', 2', 3'-gh]pentalene-
1, 4, 6, 8, 10, 12, 15, 17, 19, 21(2H, 3H, 13H, 14H)-decone,
decahydro-19b, 19c-diphenyl-, stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

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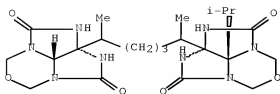
PAGE 1-B



RN 865813-89-4 HCAPLUS

CN 5H, 7H-6-Oxa-2, 3, 4a, 7a-tetraazacyclopent[cd]indene-1, 4(2H, 3H)-dione,
dihydro-7b-(1-methylethyl)-2a-[1-methyl-5-(cis-tetrahydro-1, 4-dioxo-5H, 7H-
6-oxa-2, 3, 4a, 7a-tetraazacyclopent[cd]inden-2a(7bH)-yl)hexyl]-, cis- (9CI)
(CA INDEX NAME)

Relative stereochemistry.

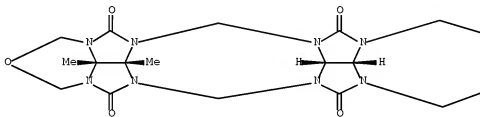


RN 865813-91-8 HCAPLUS

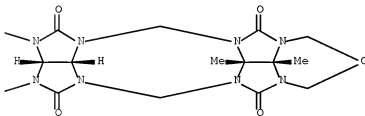
CN 1H,3H,4H,5H,6H,7H,8H,9H,10H,11H,13H,14H,15H,16H,17H,18H,19H,20H-2,12-Dioxahexadecaazabisbenzo[3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h]cycloocta[1,2,3-cd:5,6,7-c'd]dipentalene-4,6,8,10,14,16,18,20-octone, octahydro-, stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



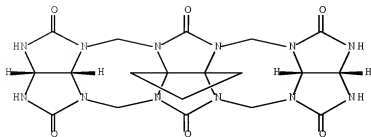
PAGE 1-B



RN 865813-92-9 HCAPLUS

CN 12H,18H-13,17-Methano-5H,6H,7H,14H-2,3,4a,5a,6a,7a,9,10,11a,13,17,18a-dodecaazabispentaleno[1',6':4,5,6]cycloocta[2,1-c:1',2'-h]pentalene-1,4,6,8,11,15(2H,3H,9H,10H,16H)-hexone, tetrahydro-, stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 865813-94-1 HCAPLUS
 CN 1H,3H,4H,5H,7H,8H-2,6-Dioxo-3a,4a,7a,8a-tetraazacyclopenta[def]fluorene-4,8-dione, 8b,8'b-(1,5-pentanediy1)bis[dihydro-8c-methyl-, (cis,cis)-(9Ci) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 3 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN

AN 2005:673299 HCAPLUS Full-text

DN 143:165454

TI Multi-nuclear metal complexes partially encapsulated by cucurbit[7-12]urils

IN Wheate, Nial Joseph; Day, Anthony Ivan; Blanch, Rodney John; Collins, John Grant

PA Unisearch Limited, Australia

SO PCT Int. Appl., 63 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005068469	A1	20050728	WO 2005-AU45	20050114 <--
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CA 2552027	A1	20050728	CA 2005-2552027	20050114 <--
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US 20080182834	A1	20080731	US 2007-586302	20071127 <--
PRAI AU 2004-900173	A	20040115	<--	

WO 2005-AU45

W 20050114 <--

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OS MARPAT 143:165454

AB The preparation of multinuclear platinum, palladium or gold complexes partially encapsulated by one or more cucurbit[7 to 12]urils is described. The invention further relates to methods for treating cancer by administering a multinuclear metal complex having antitumor activity partially encapsulated by one or more cucurbit[7 to 12]urils or their analogs. Thus, [(trans-(NH₃)₂2ClPt)2(μ-NH₂(CH₂)₃NH₂+(CH₂)₄NH₂)] partially encapsulated by cucurbit[7]uril was prepared, cytotoxicity studies performed to evaluate antitumor activity and maximum tolerated dose (MTD) measurements made.

IT 259886-50-5DP, Cucurbit[7]uril, platinum ammine complex containing
 259886-51-6DP, Cucurbit[8]uril, platinum ammine complex containing
 307001-50-9DP, Cucurbit[10]uril, platinum ammine complex containing
 387353-44-8DP, Cucurbit[9]uril, platinum ammine complex containing
 834918-58-0DP, Cucurbit[12]uril, platinum ammine complex containing
 847977-63-3DP, Cucurbit[11]uril, platinum ammine complex containing
 860295-75-6P 860295-76-7P 860295-77-8P
 860295-78-9P 860295-79-0P 860295-81-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

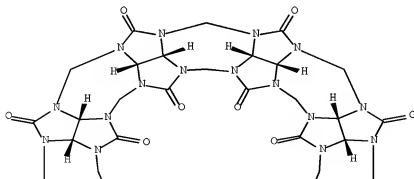
(preparation and antitumor activity of platinum ammine complex partially encapsulated by cucurbiturils)

RN 259886-50-5 HCAPLUS

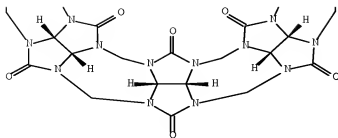
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Relative stereochemistry.

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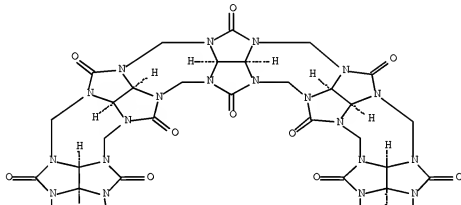
PAGE 2-A



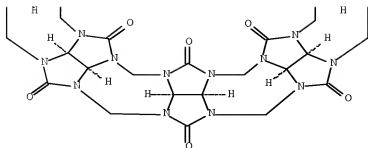
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 dotriacontazabispentaleno[1''',6''':5''',6''',7''']cycloocta[1''',
 2''',3''':3''',4''']pentaleno[1''',6''':5''',6''',7''']cycloocta[1'',2'',3
 ''':3'',4'']pentaleno[1'',6'':5,6,7]cycloocta[1,2,3-gh:1',2',3'-
 g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
 1,4,6,8,10,12,14,16,18,21,23,25,27,29,31,33-hexadecone, hexadecahydro-,
 stereoisomer (CA INDEX NAME)

Relative stereochemistry.

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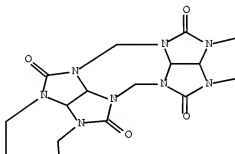


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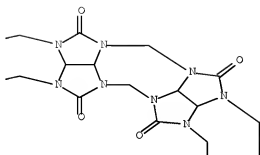


RN 307001-50-9 HCAPLUS
 CN 2,24:3,23-Dimethanotetracontaazabispentaleno[1''''''',6''''''':5''''''',6''
 ''',7''''''']cycloocta[1''''',2''''',3''''':3''''',4''''']pentaleno[1''
 ''',6''''':5''''',6''''',7''''']cycloocta[1''''',2''''',3''''':3''''',4''''']pentale
 no[1''',6''':5''',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7
]cyclooct[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-
 c'd']dipentaleneicosone, eicosahydro-, stereoisomer (CA INDEX NAME)

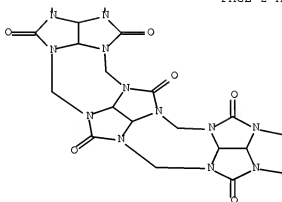
PAGE 1-A



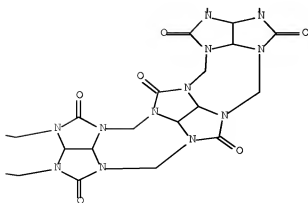
PAGE 1-B



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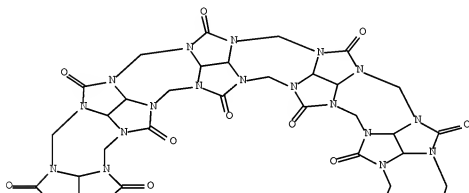


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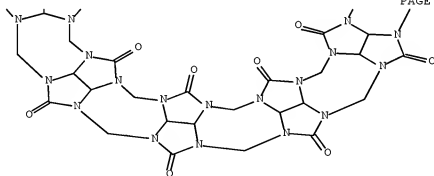


RN 387353-44-8 HCAPLUS
 CN 1H, 4H, 20H, 23H-2, 22:3, 21-Dimethano-
 2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 12a, 13a, 14a, 15a, 16a, 17a, 18a, 19a, 21, 22, 23a, 24
 a, 25a, 26a, 27a, 28a, 29a, 30a, 31a, 32a, 33a, 34a, 35a, 36a, 37a, 38a-
 hexatriacontazabispentaleno[1''''', 6''''':5''''', 6''''', 7''''']cyc
 loocta[1''''', 2''''', 3''''':3''''', 4''''']pentaleno[1''''', 6''''':5''''',
 6''''', 7''''']cycloocta[1''''', 2''''', 3''''':3''''', 4''''']pentaleno[1''''', 6''''':5''
 , 6''', 7''']cycloocta[1''', 2''', 3''':3'', 4'']pentaleno[1'', 6'':5, 6, 7]cycloocta[1, 2, 3-
 cd:1', 2', 3'-gh]pentaleneoctadecone, octadecahydro-, stereoisomer (CA
 INDEX NAME)

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RN 834918-58-0 HCAPLUS
 CN Dodeca[(dihydro-2, 5-dioxoimidazo[4, 5-d]imidazole-1, 3:4, 6 (2H, 5H)-tetrayl)-
 4, 6-bis(methylene)] (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 847977-63-3 HCAPLUS
 CN Undeca[(cis-dihydro-2, 5-dioxoimidazo[4, 5-d]imidazole-1, 3:4, 6 (2H, 5H)-

tetrayl)-4,6-bis(methylene)] (CA INDEX NAME)

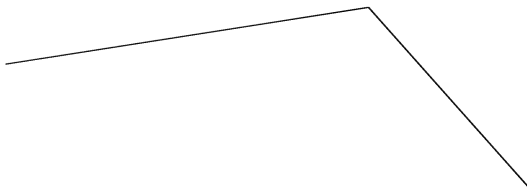
PAGE 1-B



PAGE 1-C



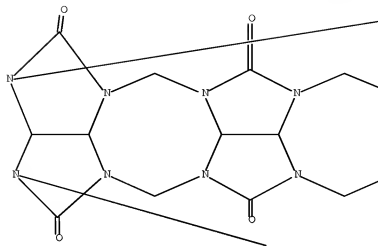
PAGE 1-D



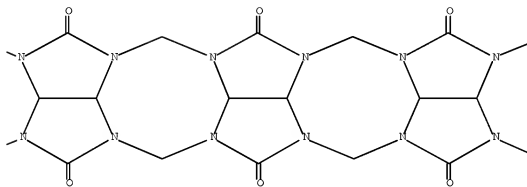
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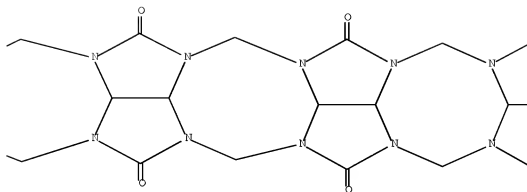
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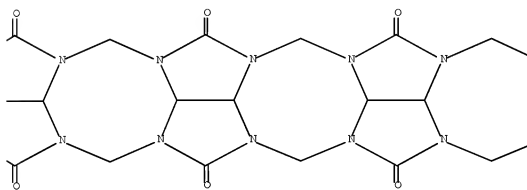
PAGE 2-B



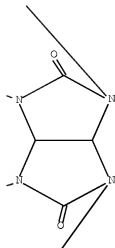
PAGE 2-C



PAGE 2-D



PAGE 2-E



PAGE 3-A

PAGE 3-B

PAGE 3-C



PAGE 3-D



PAGE 3-E



PAGE 4-C

PAGE 4-D

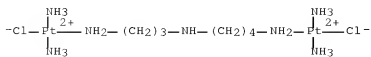
RN 860295-75-6 HCAPLUS
 CN Platinum(2+), [μ -[N-[3-(amino- κ N)propyl]-1,4-butanediamine- κ N']]tetraamminedichlorodi-, conjugate monoacid, stereoisomer, compd. with (2aa,19aa,21ba,23ba,23ca,25b.alp ha.,25ca,27ba,27ca,29ba,29ca,31ba,31c.alpha.,33ba,33ca,34ba)-hexadecahydro-2,20:3,19-dimethano-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,14a,15a,16a,17a,19,20,21a,22a,23a,24a,25a,26a,27a,28a,29a,30a,31a,32a,33a,34a-dotriacontazabispentaleno[1''''',6''''':5''''',6''''',7''''']cycloocta[1''''',2''''',3''''':3''''',4''''']pentaleno[1''''',6''''':5''''',6''''',7''''']cycloocta[1''',2'',3''':3'',4'']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,16,18,21,23,25,27,29,31,33-hexadecone (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 468066-79-7

CMF C7 H31 Cl2 N7 Pt2 . H

CCI CCS



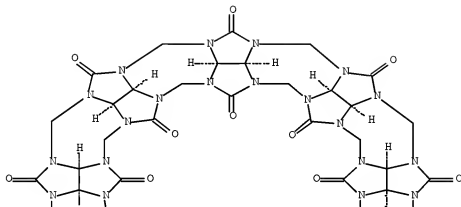
CM 2

CRN 259886-51-6

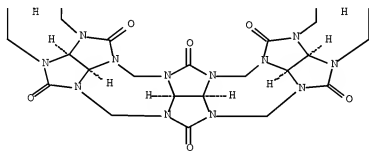
CMF C48 H48 N32 O16

Relative stereochemistry.

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RN 860295-76-7 HCAPLUS

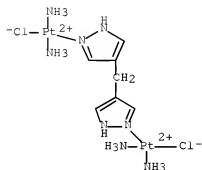
CN Platinum, tetraamminedichloro[μ-[4,4'-methylenebis[1H-pyrazole-κN2]]]di-, stereoisomer, compd. with stereoisomer of tetradecahydro-2,18:3,17-dimethano-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,14a,15a,17,18,19a,20a,21a,22a,23a,24a,25a,26a,27a,28a,29a,30a-octacosazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3''':3'',4'']pentaleno[1'',6'':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-1,4,6,8,10,12,14,16,19,21,23,25,27,29-tetradecone (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 453522-73-1

CMF C7 H20 Cl2 N8 Pt2

CCI CCS



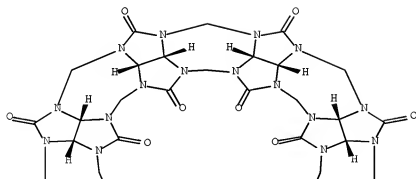
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CRN 259886-50-5

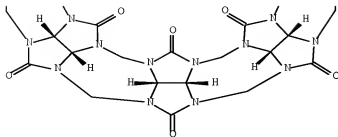
CMF C42 H42 N28 O14

Relative stereochemistry.

PAGE 1-A



PAGE 2-A



RN 860295-77-8 HCAPLUS
 CN Platinum(4+), hexaamminedichlorobis[μ-(1,6-hexanediamine-κN:κN')]tri-, compd. with stereoisomer of
 tetradecahydro-2,18:3,17-dimethano-
 2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,14a,15a,17,18,19a,20a,21a,22a,23a,24
 a,25a,26a,27a,28a,29a,30a-
 octacosazabispentaleno[1''',6''':5''',6''',7''']cycloocta[1''',2''',
 3''',4''':3''',4''']pentaleno[1''',6''':5''',6''',7''']cycloocta[1'',2'',3'':
 3'',4'']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
 1,4,6,8,10,12,14,16,19,21,23,25,27,29-tetradecone (1:1) (9CI) (CA INDEX
 NAME)

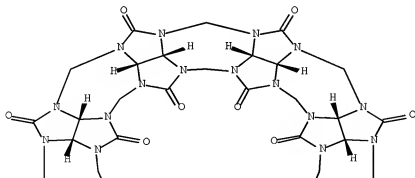
CM 1

CRN 259886-50-5

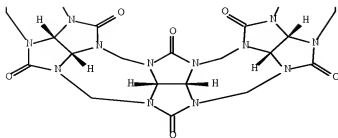
CMF C42 H42 N28 O14

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

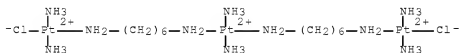


CM 2

CRN 172902-99-7

CMF C12 H50 C12 N10 Pt3

CCI CCS



RN 860295-78-9 HCAPLUS

CN Platinum(4+), hexaamminedichlorobis[μ-(1,6-hexanediamine-κN:κN')]tri-, compd. with

(2aa, 19aa, 21ba, 23ba, 23ca, 25ba, 25c.alpha

a., 27ba, 27ca, 29ba, 29ca, 31ba, 31ca, 33b.a

1pha., 33ca, 34ba)-hexadecahydro-2,20:3,19-dimethano-

2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,14a,15a,16a,17a,19,20,21a,22a,23a,24

a,25a,26a,27a,28a,29a,30a,31a,32a,33a,34a-

dotriacontazabispentaleno[1''',6''':5''',6''',7''']cycloocta[1''',

2''',3''':3''',4''']pentaleno[1''',6''':5''',6''',7''']cycloocta[1''',2''',3

''':3'',4'']pentaleno[1'',6'':5,6,7]cycloocta[1,2,3-gh:1',2',3'-

g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-

1,4,6,8,10,12,14,16,18,21,23,25,27,29,31,33-hexadecone (1:1) (9CI) (CA

INDEX NAME)

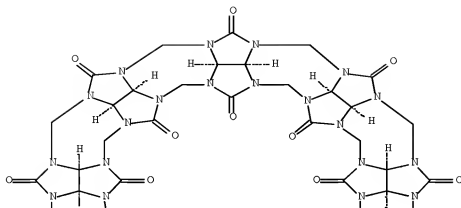
CM 1

CRN 259886-51-6

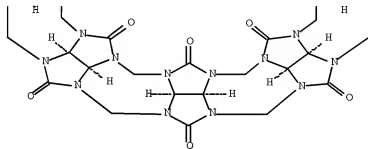
CMF C48 H48 N32 O16

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

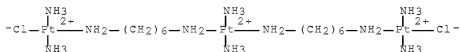


CM 2

CRN 172902-99-7

CMF C12 H50 C12 N10 Pt3

CCI CCS



RN 860295-79-0 HCAPLUS

CN Platinum(4+), hexaamminedichlorobis[μ-(1,6-hexanediamine-κN:κN')]tri-, compd. with stereoisomer of eicosahydro-2,24:3,23-dimethanotetracontaazabispentaleno[1''''',6''''':5''''',6''''',7''''']cycloocta[1''''',2''''':3''''',4''''']pentaleno[1''''',6''''':5''''',6''''',7''''']cycloocta[1''''',2''''':3''''':3''''',

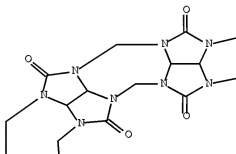
4'''pentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno
[1',6':5,6,7]cyclooct[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-
c'd']dipentaleneicosone (1:1) (9CI) (CA INDEX NAME)

CM 1

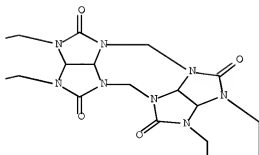
CRN 307001-50-9

CMF C60 H60 N40 O20

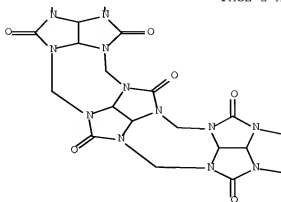
PAGE 1-A



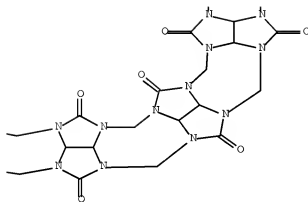
PAGE 1-B



PAGE 2-A



PAGE 2-B

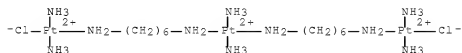


CM 2

CRN 172902-99-7

CMF C12 H50 C12 N10 Pt3

CCI CCS



RN 860295-81-4 HCAPLUS

CN Platinum(4+), hexaamminedichlorobis[μ-[4,4'-methylenebis[1H-pyrazole-kN2]]tri-, stereoisomer, compd. with stereoisomer of tetradecahydro-2,18:3,17-dimethano-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,14a,15a,17,18,19a,20a,21a,22a,23a,24a,25a,26a,27a,28a,29a,30a-octacosazabispentaleno[1''',6''':5''',6''',7''']cycloocta[1''',2'

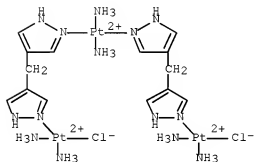
''',3''':3''',4''']pentaleno[1''',6''':5'',6'',7''']cycloocta[1'',2'',3'':
3'',4'']pentaleno[1'',6'':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
1,4,6,8,10,12,14,16,19,21,23,25,27,29-tetradecone (1:1) (9CI) (CA INDEX
NAME)

CM 1

CRN 860295-80-3

CMF C14 H34 C12 N14 Pt3

CCI CCS



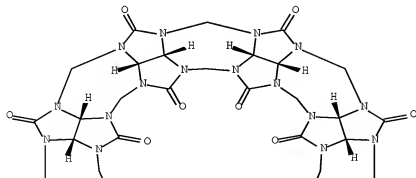
CM 2

CRN 259886-50-5

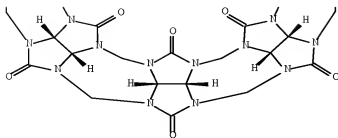
CMF C42 H42 N28 O14

Relative stereochemistry.

PAGE 1-A



PAGE 2-A



IT 960295-74-5E

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation, antitumor activity and maximum tolerated dose study of

platinum

ammine complex partially encapsulated by cucurbiturils)

RN 960295-74-5 HCAPLUS

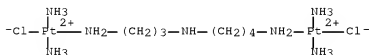
CN Platinum(2+), [μ -[N-[3-(amino-κN)propyl]-1,4-butanediamine-κN']]tetraamminedichlorodi-, conjugate monoacid, stereoisomer, compd. with stereoisomer of tetradecahydro-2,18:3,17-dimethano-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,14a,15a,17,18,19a,20a,21a,22a,23a,24a,25a,26a,27a,28a,29a,30a-octacosazabispentaleno[1''',6''':5''',6''',7''']cycloocta[1''',2''':3''',4''':3''',4''']pentaleno[1''',6''':5''',6''',7''']cycloocta[1'',2'',3'':3'',4'']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-1,4,6,8,10,12,14,16,19,21,23,25,27,29-tetradecone (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 468066-79-7

CMF C7 H31 Cl2 N7 Pt2 . H

CCI CCS



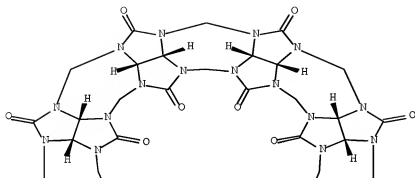
CM 2

CRN 259886-50-5

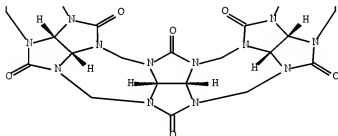
CMF C42 H42 N28 O14

Relative stereochemistry.

PAGE 1-A



PAGE 2-A



OSC.G 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)
 RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 4 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN

AN 2005:532408 HCAPLUS [Full-text](#)

DN 144:149957

TI Investigation of Host-Guest Compounds of Cucurbit[n=5-8]uril with Some
 Ortho Aminopyridines and Bispyridine

AU Fu, Hai-Yan; Xue, Sai-Feng; Zhu, Qian-Jiang; Tao, Zhu; Zhang, Jian-Xin;
 Day, Anthony I.

CS Institute of Applied Chemistry, Guizhou University, Guiyang, 550025, Peop.
 Rep. China

SO Journal of Inclusion Phenomena and Macrocyclic Chemistry (2005),
 52(1-2), 101-107

CODEN: JIPCF5; ISSN: 1388-3127

PB Springer

DT Journal

LA English

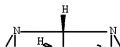
AB Host-guest complexes of cucurbit[n=5-8]uril and some examples of ortho
 substituted pyridines or aminopyridines were examined by 1H NMR spectroscopy.
 Portal binding of two ortho aminopyridine free bases, by cucurbit[5]uril, was

observed in 1H NMR spectra. Combined cavity and portal binding in cucurbit[6]uril were observed for both the free base 2-aminomethylpyridine, ampy, the HCl salt, ampy·1HCl, and the salt of 2,2'-bispyridine, bpy·1HCl. Two novel complexes were formed with cucurbit[6]uril. The free base ampy as a dual occupant, formed a 2:1 complex, and bpy·1HCl formed a stable asym. 1:1 complex. Only portal binding of 2,6-bis(aminomethyl)pyridine and its salts was observed for cucurbit[6]uril. Fast exchange of the free base and pyridineammonium salts was observed for cucurbit[7-8]uril.

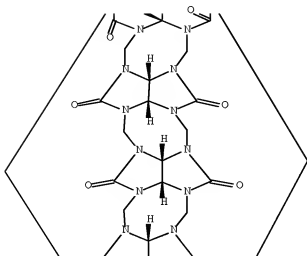
IT 259886-49-2, Cucurbit[5]uril
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PROC (Process)
 (competitive binding of cucurbit[5]uril by K⁺ and aminopyridines; host-guest compds. of cucurbit[n=5-8]uril with some o-aminopyridines and bispyridine)
 RN 259886-49-2 HCAPLUS
 CN 1H,4H,12H,15H-2,14:3,13-Dimethano-5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-eicosazaabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3''':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-1,4,6,8,10,12,15,17,19,21-decone, decahydro-, stereoisomer (CA INDEX NAME)

Relative stereochemistry.

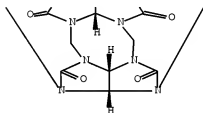
PAGE 1-A



PAGE 2-A



PAGE 3-A



IT 873852-54-1 873852-55-2 873852-56-3

873852-57-4 873852-58-5

RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
 (inclusion complex; host-guest compds. of cucurbit[n=5-8]uril with some
 o-aminopyridines and bispyridine)

RN 873852-54-1 HCAPLUS

CN 1H, 4H, 14H, 17H-2, 16:3, 15-Dimethano-
 5H, 6H, 7H, 8H, 9H, 10H, 11H, 12H, 13H, 18H, 19H, 20H, 21H, 22H, 23H, 24H, 25H, 26H-
 2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 12a, 13a, 15, 16, 17a, 18a, 19a, 20a, 21a, 22a, 23a, 24
 a, 25a, 26a-tetracosazabispentaleno[1''', 6''' : 5'', 6'', 7''']cycloocta[1'', 2''
 , 3''' : 3', 4']pentaleno[1', 6' : 5, 6, 7]cycloocta[1, 2, 3-gh : 1', 2', 3'-
 g'h']cycloocta[1, 2, 3-cd : 5, 6, 7-c'd']dipentalene-
 1, 4, 6, 8, 10, 12, 14, 17, 19, 21, 23, 25-dodecone, dodecahydro-, stereoisomer,
 compd. with 2-pyridinemethanamine (1:1) (9CI) (CA INDEX NAME)

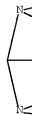
CM 1

CRN 283175-97-3

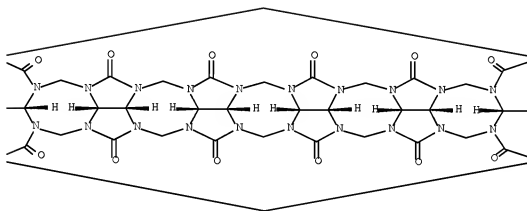
CMF C36 H36 N24 O12

Relative stereochemistry.

PAGE 1-A



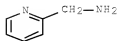
PAGE 1-B



PAGE 1-C



CRN 3731-51-9
CMF C6 H8 N2



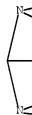
RN 873852-55-2 HCAPLUS
CN 1H, 4H, 14H, 17H-2, 16:3, 15-Dimethano-
5H, 6H, 7H, 8H, 9H, 10H, 11H, 12H, 13H, 18H, 19H, 20H, 21H, 22H, 23H, 24H, 25H, 26H-
2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 12a, 13a, 15, 16, 17a, 18a, 19a, 20a, 21a, 22a, 23a, 24
a, 25a, 26a-tetracosazabispentaleno[1'', 6'':5'', 6'':7'']cycloocta[1'', 2''
, 3'':3', 4']pentaleno[1', 6':5, 6, 7]cycloocta[1, 2, 3-gh:1', 2', 3'-
g'h']cycloocta[1, 2, 3-cd:5, 6, 7-c'd']dipentalene-
1, 4, 6, 8, 10, 12, 14, 17, 19, 21, 23, 25-dodecone, dodecahydro-, stereoisomer,
compd. with 2-pyridinemethanamine (1:2) (9CI) (CA INDEX NAME)

CM 1

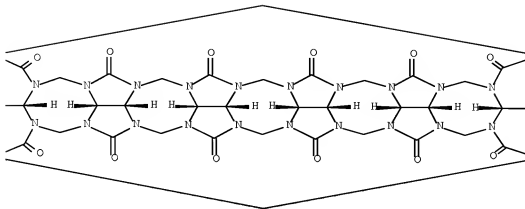
CRN 283175-97-3
CMF C36 H36 N24 O12

Relative stereochemistry.

PAGE 1-A



PAGE 1-B



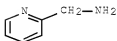
PAGE 1-C



CM 2

CRN 3731-51-9

CMF C6 H8 N2



RN 873852-56-3 HCAPLUS

CN 1H, 4H, 14H, 17H-2, 16:3, 15-Dimethano-
 5H, 6H, 7H, 8H, 9H, 10H, 11H, 12H, 13H, 18H, 19H, 20H, 21H, 22H, 23H, 24H, 25H, 26H-
 2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 12a, 13a, 15, 16, 17a, 18a, 19a, 20a, 21a, 22a, 23a, 24
 a, 25a, 26a-tetracosazabispentaleno[1''', 6''' : 5'', 6'', 7''']cycloocta[1'', 2''
 , 3''' : 3', 4']pentaleno[1', 6' : 5, 6, 7]cycloocta[1, 2, 3-gh:1', 2', 3'-
 g'h']cycloocta[1, 2, 3-cd:5, 6, 7-c'd']dipentalene-
 1, 4, 6, 8, 10, 12, 14, 17, 19, 21, 23, 25-dodecone, dodecahydro-, stereoisomer,
 compd. with 2,2'-bipyridine monohydrochloride (1:1) (9CI) (CA INDEX NAME)

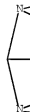
CM 1

CRN 283175-97-3

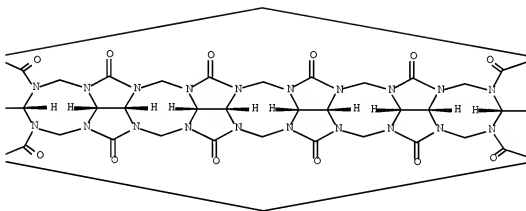
CMF C36 H36 N24 O12

Relative stereochemistry.

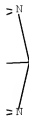
PAGE 1-A



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PAGE 1-C



CM 2

CRN 65520-13-0

CMF C10 H8 N2 . C1 H



● HCl

RN 873852-57-4 HCAPLUS

CN 1H, 4H, 14H, 17H-2, 16:3, 15-Dimethano-
 5H, 6H, 7H, 8H, 9H, 10H, 11H, 12H, 13H, 18H, 19H, 20H, 21H, 22H, 23H, 24H, 25H, 26H-
 2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 12a, 13a, 15, 16, 17a, 18a, 19a, 20a, 21a, 22a, 23a, 24
 a, 25a, 26a-tetracosazabispentaleno[1''', 6''' : 5'', 6'', 7'']cycloocta[1'', 2''
 , 3''' : 3', 4']pentaleno[1', 6' : 5, 6, 7]cycloocta[1, 2, 3-gh:1', 2', 3'-
 g'h']cycloocta[1, 2, 3-cd:5, 6, 7-c'd']dipentalene-
 1, 4, 6, 8, 10, 12, 14, 17, 19, 21, 23, 25-dodecone, dodecahydro-, stereoisomer,
 compd. with pyridine hydrochloride (9CI) (CA INDEX NAME)

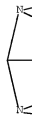
CM 1

CRN 283175-97-3

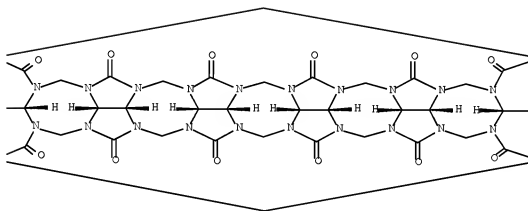
CMF C36 H36 N24 O12

Relative stereochemistry.

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PAGE 1-B



PAGE 1-C



CRN 628-13-7
CMF C5 H5 N . Cl H



● HCl

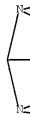
RN 873852-58-5 HCAPLUS
CN 1H, 4H, 14H, 17H-2, 16:3, 15-Dimethano-
5H, 6H, 7H, 8H, 9H, 10H, 11H, 12H, 13H, 18H, 19H, 20H, 21H, 22H, 23H, 24H, 25H, 26H-
2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 12a, 13a, 15, 16, 17a, 18a, 19a, 20a, 21a, 22a, 23a, 24
a, 25a, 26a-tetracosazabispentaleno[1''', 6''' : 5'', 6'', 7'']cycloocta[1'', 2''
, 3''' : 3', 4']pentaleno[1', 6' : 5, 6, 7]cycloocta[1, 2, 3-gh:1', 2', 3'-
g'h']cycloocta[1, 2, 3-cd:5, 6, 7-c'd']dipentalene-
1, 4, 6, 8, 10, 12, 14, 17, 19, 21, 23, 25-dodecone, dodecahydro-, stereoisomer,
compd. with 2-pyridineethanamine monohydrochloride (9CI) (CA INDEX NAME)

CM 1

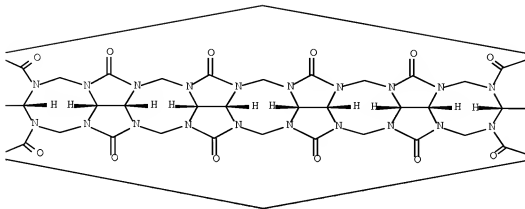
CRN 283175-97-3
CMF C36 H36 N24 O12

Relative stereochemistry.

PAGE 1-A



PAGE 1-B



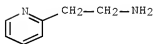
PAGE 1-C



CM 2

CRN 3668-52-8

CMF C7 H10 N2 . C1 H



● HCl

IT 259886-51-6, Cucurbit[8]uril

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PROC (Process)

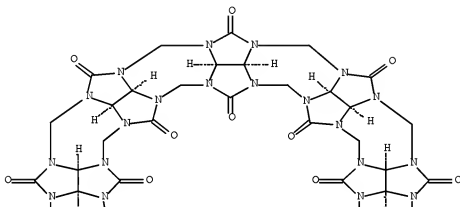
(solubilization by bipyridine hydrochloride; host-guest compds. of cucurbit[n=5-8]uril with some o-aminopyridines and bispyridine)

RN 259886-51-6 HCAPLUS

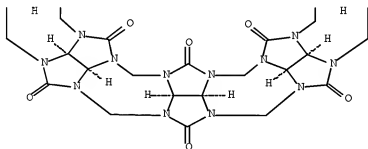
CN 2,20:3,19-Dimethano-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,14a,15a,16a,17a,19,20,21a,22a,23a,24a,25a,26a,27a,28a,29a,30a,31a,32a,33a,34a-dotriacontazabispentaleno[1''',6''':5''',6''',7''']cycloocta[1''',2''',3''':3'',4'']pentaleno[1''',6''':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,16,18,21,23,25,27,29,31,33-hexadecone, hexadecahydro-, stereoisomer (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A



OSC.G 20 THERE ARE 20 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)
 RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 5 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN

AN 2005:260070 HCAPLUS [Full-text](#)

DN 142:336358

TI Method for preparing cucurbiturils

IN Day, Anthony Ivan; Arnold, Alan Peter; Blanch, Rodney John

PA Unisearch Limited, Australia

SO PCT Int. Appl., 58 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005026168	A1	20050324	WO 2004-AU1232	20040910 <--
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2004272121	A1	20050324	AU 2004-272121	20040910 <--
	CA 2537843	A1	20050324	CA 2004-2537843	20040910 <--
	EP 1668012	A1	20060614	EP 2004-761268	20040910 <--
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	JP 2007505046	T	20070308	JP 2006-525577	20040910 <--
	KR 2006119979	A	20061124	KR 2006-705066	20060311 <--
	US 20070066818	A1	20070322	US 2006-571707	20060313 <--
	US 7501523	B2	20090310		
	IN 2006DN01397	A	20070803	IN 2006-DN1397	20060314 <--
PRAI	AU 2003-905037	A	20030912	<--	
	WO 2004-AU1232	W	20040910	<--	

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OS CASREACT 142:336358; MARPAT 142:336358

AB The invention relates to a method for preparing cucurbiturils. The method comprises reacting an oligomer consisting of 2 to 11 linked glycolurils or glycoluril analogs with one or more compds. selected from glycoluril, glycoluril analogs and/or oligomers of glycoluril or glycoluril analogs, in the presence of an acid, to form a cucurbituril. The method can be used to prepare variably substituted cucurbiturils having specific substituted units at specific locations in the cucurbituril. Thus, dimethylcucurbit[1,4]uril was obtained by treating the formaldehyde diether of dimethylglycoluril with the diether of glycoluril and paraformaldehyde in concentrated HCl.

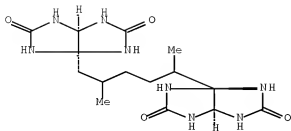
IT 848440-40-4 848440-50-6

RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of cucurbiturils as complexing agents)

RN 848440-40-4 HCAPLUS

CN Imidazo[4,5-d]imidazole-2,5(1H,3H)-dione,
 3a,3'a-(1,4-dimethyl-1,5-pentanediy)bis[tetrahydro-, (cis,cis)- (9CI)
 (CA INDEX NAME)

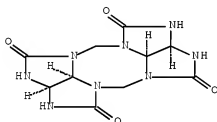
Relative stereochemistry.



RN 848440-50-6 HCAPLUS

CN 5H,10H-2,3,4a,5a,7,8,9a,10a-Octaazacycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,9(2H,3H,7H,8H)-tetrone, tetrahydro-, stereoisomer (CA INDEX NAME)

Relative stereochemistry.



IT 948440-48-2P

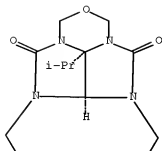
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cucurbiturils as complexing agents)

RN 848440-48-2 HCAPLUS

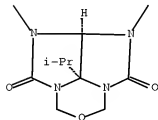
CN 1H,3H,4H,5H,6H,7H,9H,10H,11H,12H-2,8-Dioxa-3a,4a,5a,6a,9a,10a,11a,12a-octaazadibenzo[gh,g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-4,6,10,12-tetrone, tetrahydro-10c,12b-bis(1-methylethyl)-, stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

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IT 263175-97-3DP, Cucurbit[6]uril, derivs. 569359-77-5P

648440-49-3P 648440-51-7P 648440-52-8P

648440-55-1P 648440-56-2P 648440-57-3P

648440-58-4P 648440-59-5P 648440-61-9P

648491-90-7P 648491-91-8P 648491-92-9P

648491-93-0P 665813-91-8P 665813-92-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of cucurbiturils as complexing agents)

RN 283175-97-3 HCAPLUS

CN 1H, 4H, 14H, 17H-2, 16:3, 15-Dimethano-

5H, 6H, 7H, 8H, 9H, 10H, 11H, 12H, 13H, 18H, 19H, 20H, 21H, 22H, 23H, 24H, 25H, 26H-

2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 12a, 13a, 15, 16, 17a, 18a, 19a, 20a, 21a, 22a, 23a, 24

a, 25a, 26a-tetracosazabispentaleno[1'', 6'':5'', 6'', 7'']cycloocta[1'', 2'',

3'':3', 4']pentaleno[1', 6':5, 6, 7]cycloocta[1, 2, 3-gh:1', 2', 3'-

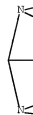
g'h']cycloocta[1, 2, 3-cd:5, 6, 7-c'd']dipentalene-

1, 4, 6, 8, 10, 12, 14, 17, 19, 21, 23, 25-dodecone, dodecahydro-, stereoisomer (CA

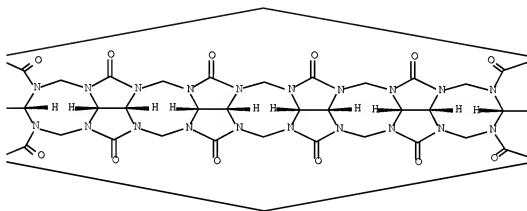
INDEX NAME)

Relative stereochemistry.

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RN 569359-77-9 HCAPLUS
 CN 1H, 4H, 12H, 15H-2, 14:3, 13-Dimethano-
 5H, 6H, 7H, 8H, 9H, 10H, 11H, 16H, 17H, 18H, 19H, 20H, 21H, 22H-

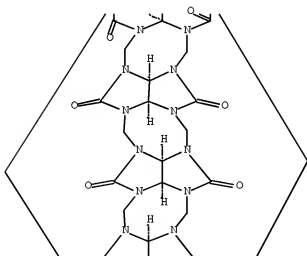
2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-eicosazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-1,4,6,8,10,12,15,17,19,21-decone, decahydro-2a,22b-dimethyl-, stereoisomer (CA INDEX NAME)

Relative stereochemistry.

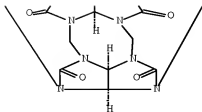
PAGE 1-A



PAGE 2-A



PAGE 3-A

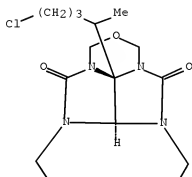


RN 848440-49-3 HCAPLUS

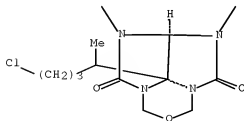
CN 1H, 3H, 4H, 5H, 6H, 7H, 9H, 10H, 11H, 12H-2, 8-Dioxa-3a, 4a, 5a, 6a, 9a, 10a, 11a, 12a-octaazadibenzo[gh, g'h']cycloocta[1, 2, 3-cd:5, 6, 7-c'd']dipentalene-4, 6, 10, 12-tetrone, 10c, 12b-bis(4-chloro-1-methylbutyl)tetrahydro-, stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

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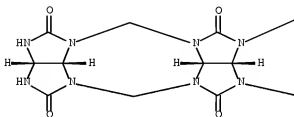
RN 848440-51-7 HCAPLUS

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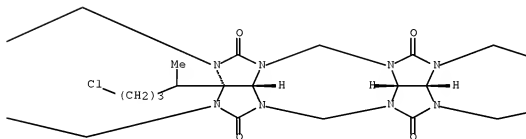
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1,4,6,8,10,12,15,17,19,21(2H,3H,13H,14H)-decone,
19b-(4-chloro-1-methylbutyl)decahydro-, stereoisomer (9CI) (CA INDEX
NAME)

Relative stereochemistry.

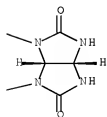
PAGE 1-A



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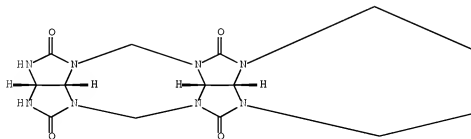


RN 848440-52-8 HCAPLUS
CN 5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-
2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-
Eicosaazabispentaleno[1'',6'':5',6',7']cycloocta[1'',2'',3'':3',4']pe
ntaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
1,4,6,8,10,12,15,17,19,21(2H,3H,13H,14H)-decone,

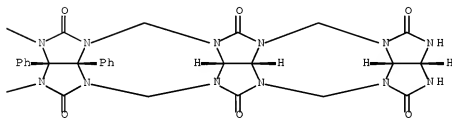
decahydro-19b,19c-diphenyl-, stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

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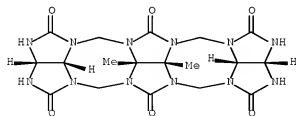
PAGE 1-B



RN 848440-55-1 HCAPLUS

CN 5H,6H,7H,12H,13H,14H-2,3,4a,5a,6a,7a,9,10,11a,12a,13a,14a-Dodecaazabispentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-1,4,6,8,11,13(2H,3H,9H,10H)-hexone, hexahydro-13b,13c-dimethyl-, stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.



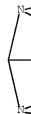
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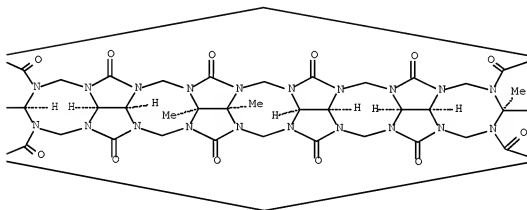
g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
 1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
 dodecahydro-2a,21b,21c,26b-tetramethyl-, stereoisomer (CA INDEX NAME)

Relative stereochemistry.

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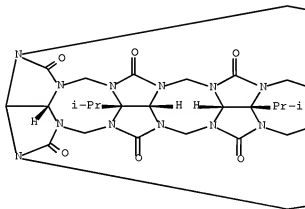
PAGE 1-C



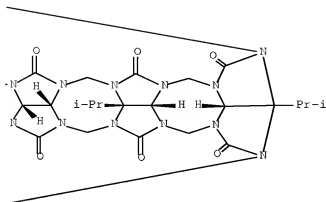
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 a, 25a, 26a-tetracosazabispentaleno[1''', 6''' : 5'', 6'', 7'']cycloocta[1'', 2''
 , 3''' : 3', 4']pentaleno[1', 6' : 5, 6, 7]cycloocta[1, 2, 3-gh:1', 2', 3'-
 g'h']cycloocta[1, 2, 3-cd:5, 6, 7-c'd']dipentalene-
 1, 4, 6, 8, 10, 12, 14, 17, 19, 21, 23, 25-dodecone,
 dodecahydro-2a, 19c, 21b, 25c-tetrakis(1-methylethyl)-, stereoisomer (9CI)
 (CA INDEX NAME)

Relative stereochemistry.

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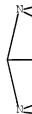
PAGE 1-B



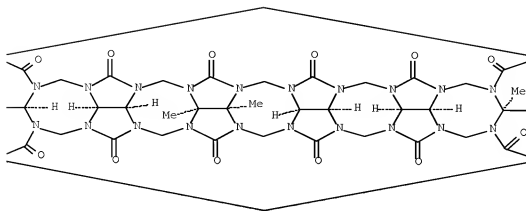
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 a, 25a, 26a-tetracosazabispentaleno[1'', 6'':5'', 6'', 7'']cycloocta[1'', 2'',
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 g'h']cycloocta[1, 2, 3-cd:5, 6, 7-c'd']dipentalene-
 1, 4, 6, 8, 10, 12, 14, 17, 19, 21, 23, 25-dodecone,
 dodecahydro-2a, 21b, 21c-trimethyl-26b-phenyl-, stereoisomer (9CI) (CA
 INDEX NAME)

Relative stereochemistry.

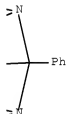
PAGE 1-A



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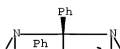
PAGE 1-C



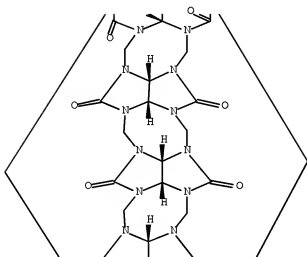
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 2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-
 eicosaazabispentaleno[1'',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pe
 ntaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
 1,4,6,8,10,12,15,17,19,21-decone, decahydro-2a,22b-diphenyl-, stereoisomer
 (9CI) (CA INDEX NAME)

Relative stereochemistry.

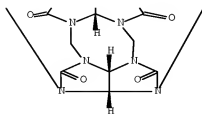
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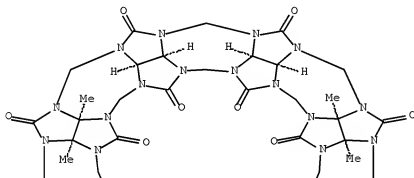
PAGE 3-A



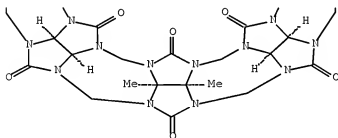
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Relative stereochemistry.

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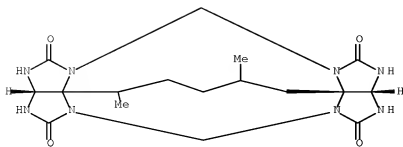


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RN 848491-90-7 HCAPLUS
 CN 2H,9H-1,13-Methano-7H,14H-diimidazo[4',5':4,5]imidazo[1,5-c:5',1'-j][1,3]diazecine-2,5,9,12-tetrone, decahydro-14,17-dimethyl- (CA INDEX NAME)

Relative stereochemistry.



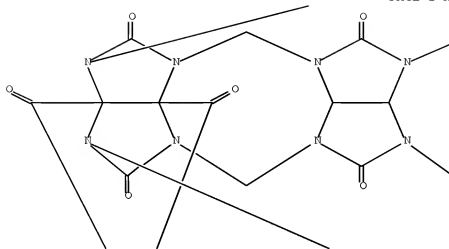
RN 848491-91-8 HCAPLUS
 CN 1H, 4H, 14H, 17H-2a, 26b:21b, 21c-Bis(methaniminomethano)-2,16:3,15-dimethano-5H, 6H, 7H, 8H, 9H, 10H, 11H, 12H, 13H, 18H, 19H, 20H, 21H, 22H, 23H, 24H, 25H, 26H-2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 12a, 13a, 15, 16, 17a, 18a, 19a, 20a, 21a, 22a, 23a, 24a, 25a, 26a-tetracosazabispentaleno[1'', 6'':5'', 6'', 7'']cycloocta[1'', 2'', 3'':3', 4']pentaleno[1', 6':5, 6, 7]cycloocta[1, 2, 3-gh:1', 2', 3'-g'h']cycloocta[1, 2, 3-cd:5, 6, 7-c'd']dipentalene-1, 4, 6, 8, 10, 12, 14, 17, 19, 21, 23, 25, 27, 29, 30, 32-hexadecone, 28, 31-dibutyloctahydro-, stereoisomer (9CI) (CA INDEX NAME)

PAGE 1-A

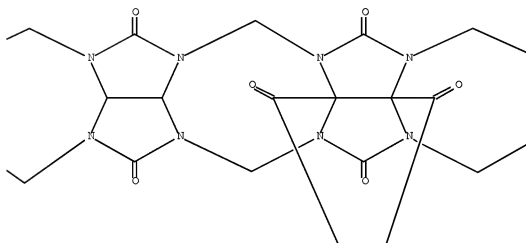
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

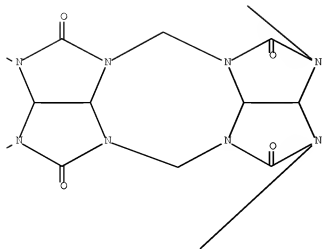
PAGE 2-A



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PAGE 2-C



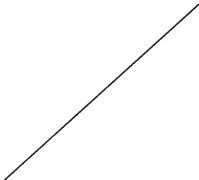
PAGE 3-A



PAGE 3-B



PAGE 3-C



PAGE 4-B

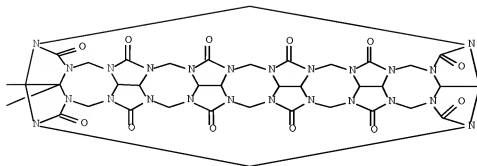


RN 848491-92-9 HCAPLUS
 CN 1H, 4H, 14H, 17H-2, 16:3, 15-Dimethano-
 5H, 6H, 7H, 8H, 9H, 10H, 11H, 12H, 13H, 18H, 19H, 20H, 21H, 22H, 23H, 24H, 25H, 26H-
 2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 12a, 13a, 15, 16, 17a, 18a, 19a, 20a, 21a, 22a, 23a, 24
 a, 25a, 26a-tetracosazabispentaleno[1'', 6''':5'', 6'', 7'']cycloocta[1'', 2''
 , 3'':3', 4']pentaleno[1', 6':5, 6, 7]cycloocta[1, 2, 3-gh:1', 2', 3'-
 g'h']cycloocta[1, 2, 3-cd:5, 6, 7-c'd']dipentalene-
 1, 4, 6, 8, 10, 12, 14, 17, 19, 21, 23, 25-dodecone, dodecahydro-2a, 21b(or
 2a, 21c)-bis(4-iodophenyl)-21c, 26b(or 21b, 26b)-dimethyl-, stereoisomer
 (9CI) (CA INDEX NAME)

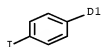
PAGE 1-A



PAGE 1-B



PAGE 2-A



D1-Me

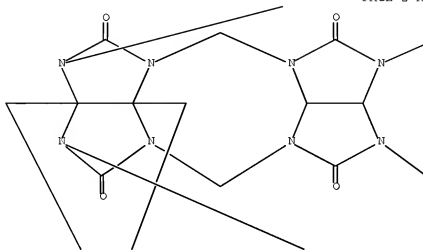
RN 848491-93-0 HCAPLUS
 CN 1H, 4H, 14H, 17H-2, 16:3, 15-Dimethano-2a, 26b:21b, 21c-dipropano-
 5H, 6H, 7H, 8H, 9H, 10H, 11H, 12H, 13H, 18H, 19H, 20H, 21H, 22H, 23H, 24H, 25H, 26H-
 2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 12a, 13a, 15, 16, 17a, 18a, 19a, 20a, 21a, 22a, 23a, 24
 a, 25a, 26a-tetracosazaabispentaleno[1''', 6''':5'', 6'', 7'']cycloocta[1'', 2'',
 3''':3', 4']pentaleno[1', 6':5, 6, 7]cycloocta[1, 2, 3-gh:1', 2', 3'-
 g'h']cycloocta[1, 2, 3-cd:5, 6, 7-c'd']dipentalene-
 1, 4, 6, 8, 10, 12, 14, 17, 19, 21, 23, 25-dodecone, octahydro-, stereoisomer (9CI)
 (CA INDEX NAME)

PAGE 1-A

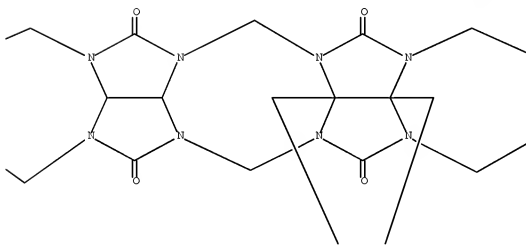
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

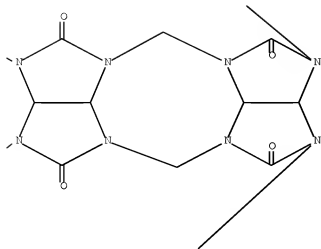
PAGE 2-A



PAGE 2-B



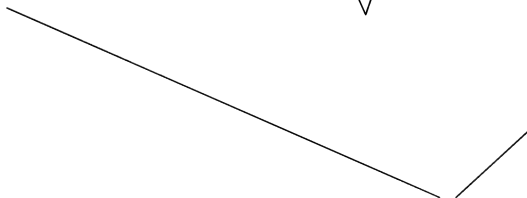
PAGE 2-C



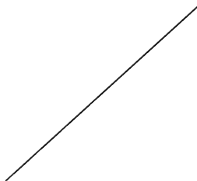
PAGE 3-A



PAGE 3-B



PAGE 3-C

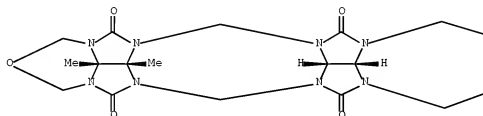


PAGE 4-B

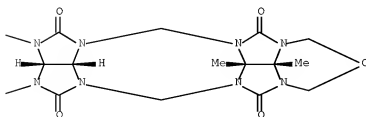
RN 865813-91-8 HCAPLUS
 CN 1H, 3H, 4H, 5H, 6H, 7H, 8H, 9H, 10H, 11H, 13H, 14H, 15H, 16H, 17H, 18H, 19H, 20H-2, 12-Diox-
 3a, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 13a, 14a, 15a, 16a, 17a, 18a, 19a, 20a-
 hexadecaazabisbenzo[3', 4']pentaleno[1', 6':5, 6, 7]cycloocta[1, 2, 3-
 gh:1', 2', 3'-g'h']cycloocta[1, 2, 3-cd:5, 6, 7-c'd']dipentalene-
 4, 6, 8, 10, 14, 16, 18, 20-octone, octahydro-, stereoisomer (9CI) (CA INDEX
 NAME)

Relative stereochemistry.

PAGE 1-A



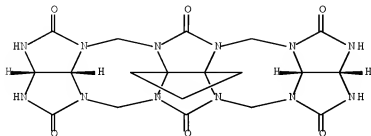
PAGE 1-B



RN 865813-92-9 HCAPLUS

CN 12H, 18H-13, 17-Methano-5H, 6H, 7H, 14H-2, 3, 4a, 5a, 6a, 7a, 9, 10, 11a, 13, 17, 18a-dodecaazabispentaleno[1', 6':4, 5, 6]cycloocta[2, 1-c:1', 2'-h]pentalene-1, 4, 6, 8, 11, 15(2H, 3H, 9H, 10H, 16H)-hexone, tetrahydro-, stereoisomer (9CI)
(CA INDEX NAME)

Relative stereochemistry.



OSC.G 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 6 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN

AN 2004:684964 HCAPLUS [Full-text](#)

DN 143:7687

TI Synthesis of a symmetrical tetrasubstituted cucurbit[6]uril and its host-guest inclusion complex with 2,2'-bipyridine

AU Zhao, Yunjie; Xue, Saifeng; Zhu, Qianjiang; Tao, Zhu; Zhang, Jianxin; Wei, Zhanbin; Long, Lasheng; Hu, Maolin; Xiao, Hongping; Day, Anthony J.

CS Institute of Applied Chemistry, Guizhou University, Guiyang, 550025, Peop. Rep. China

SO Chinese Science Bulletin (2004), 49(11), 1111-1116

CODEN: CSBUEF; ISSN: 1001-6538

PB Science in China Press

DT Journal

LA English

OS CASREACT 143:7687

AB Synthesis of a sym. tetramethylcucurbit[6]uril (TMeQ[6]) has been achieved by using the diether of dimethylglycoluril and the dimer of glycoluril. The structure of TMeQ[6] has been determined by single crystal X-ray diffraction, ¹H NMR spectroscopy and ESMS. The ¹H NMR spectra of 2,2'-bipyridine added to TMeQ[6] reveal that the host-guest inclusion complex was easily formed.

IT 848440-56-2P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

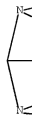
(preparation and crystal structure of sym. tetrasubstituted cucurbit[6]uril and its host-guest inclusion complex with bipyridine)

RN 848440-56-2 HCAPLUS

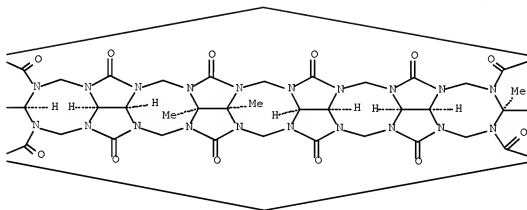
CN 1H, 4H, 14H, 17H-2, 16:3, 15-Dimethano-5H, 6H, 7H, 8H, 9H, 10H, 11H, 12H, 13H, 18H, 19H, 20H, 21H, 22H, 23H, 24H, 25H, 26H-2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 12a, 13a, 15, 16, 17a, 18a, 19a, 20a, 21a, 22a, 23a, 24a, 25a, 26a-tetracosazabispentaleno[1'', 6'':5'', 6'', 7'']cycloocta[1'', 2'', 3'':3', 4']pentaleno[1', 6':5, 6, 7]cycloocta[1, 2, 3-gh:1', 2', 3'-g'h']cycloocta[1, 2, 3-cd:5, 6, 7-c'd']dipentalene-1, 4, 6, 8, 10, 12, 14, 17, 19, 21, 23, 25-dodecone, dodecahydro-2a, 21b, 21c, 26b-tetramethyl-, stereoisomer (CA INDEX NAME)

Relative stereochemistry.

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PAGE 1-B



PAGE 1-C



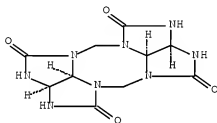
IT 648440-50-6

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and crystal structure of sym. tetrasubstituted cucurbit[6]uril
and its host-guest inclusion complex with bipyridine)

RN 848440-50-6 HCAPLUS

CN 5H,10H-2,3,4a,5a,7,8,9a,10a-Octaazacycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,9(2H,3H,7H,8H)-tetrone, tetrahydro-, stereoisomer (CA INDEX NAME)

Relative stereochemistry.



OSC.G 43 THERE ARE 43 CAPLUS RECORDS THAT CITE THIS RECORD (43 CITINGS)
RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 7 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN

AN 2004:460911 HCAPLUS Full-text

DN 141:199653

TI Multi-nuclear platinum complexes encapsulated in cucurbit[n]uril as an approach to reduce toxicity in cancer treatment

AU Wheate, Nial J.; Day, Anthony I.; Blanch, Rodney J.; Arnold, Alan P.; Cullinane, Carleen; Collins, J. Grant

CS Department of Defence, Joint Health Support Agency, Campbell, Australia

SO Chemical Communications (Cambridge, United Kingdom) (2004),
(12), 1424-1425

CODEN: CHCOFS; ISSN: 1359-7345

PB Royal Society of Chemistry

DT Journal

LA English

AB The dinuclear platinum complex trans-[[Pt(NH₃)₂Cl]₂μ-dpzm]₂ (di-Pt) binds inside cucurbit[7]uril with slow exchange kinetics which does not significantly affect the cytotoxicity of the dinuclear complex but reactivity at the platinum center is reduced.

IT 259886-50-5D, Cucurbit[7]uril, complexes with multinuclear platinum compds.

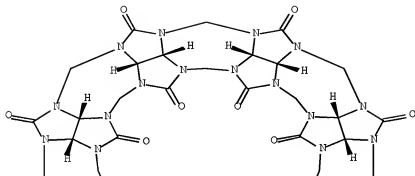
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (multinuclear platinum complexes encapsulated in cucurbit[n]uril as approach to reduce toxicity in cancer treatment)

RN 259886-50-5 HCAPLUS

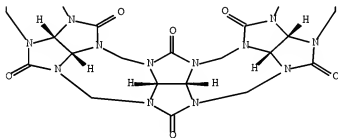
CN 2,18:3,17-Dimethano-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,14a,15a,17,18,19a,20a,21a,22a,23a,24a,25a,26a,27a,28a,29a,30a-octacosazaabipentaleno[1''',6''',5''',5''',6''',6''',7''']cycloocta[1''',2''',3''',3''',3''',4''']pentaleno[1''',6''',5''',6''',6''',7''']cycloocta[1''',2''',3''',4''']pentaleno[1'',6'':5,6',7']cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-1,4,6,8,10,12,14,16,19,21,23,25,27,29-tetradecone, tetradecahydro-, stereoisomer (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



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OSC.G 45 THERE ARE 45 CAPLUS RECORDS THAT CITE THIS RECORD (45 CITINGS)
 RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 8 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN

AN 2003:726647 HCAPLUS [Full-text](#)

DN 139:364581

TI Host Properties of Cucurbit[7]uril: Fluorescence Enhancement of Anilinonaphthalene Sulfonates

AU Wagner, Brian D.; Stojanovic, Natasa; Day, Anthony I.; Blanch, Rodney J.

CS Department of Chemistry, University of Prince Edward Island, Charlottetown, PE, C1A 4P3, Can.

SO Journal of Physical Chemistry B (2003), 107(39), 10741-10746
 CODEN: JPCBFK; ISSN: 1520-6106

PB American Chemical Society

DT Journal

LA English

AB This work describes the fluorescence enhancement of the probes 2,6- and 1,8-ANS via complexation with the macrocyclic host cucurbit[7]uril (Q7). The

association of these two guests with the Q7 host has been studied using fluorescence, ¹H NMR spectroscopy, and mol. modeling. In the case of 2,6-ANS, 1:1 inclusion complexes are formed via inclusion of the Ph moiety into the Q7 cavity (as confirmed by NMR), with a large fluorescence enhancement of a factor of 25 ± 3 and an association constant of $600 \pm 150 \text{ M}^{-1}$. These values are significantly larger than those reported in the literature for 2,6-ANS inclusion into cucurbit[6]uril (Q6); for example, the association constant is larger by over an order of magnitude, indicating the superior host abilities of Q7 as compared to its smaller homolog. These results are significant, as they provide the first direct comparison of the host abilities of Q6 and Q7. In the case of 1,8-ANS, very large fluorescence enhancement was also observed upon addition of Q7. The enhancement as a function of Q7 concentration indicated the formation of a 2:1 host:guest complex. However, host-guest inclusion was not observed via NMR. Thus, a 2:1 complex where 1,8-ANS is sandwiched between the outer surface of two Q7 mols. is proposed. Such complexation is supported by semiempirical PM3 calcs., and the resulting minimized structures are reminiscent of the structure of the solid exclusion compound of 1,8-ANS and Q6 previously reported in the literature.

IT 620161-23-1 620161-24-2

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(inclusion complex; fluorescence enhancement of anilidonaphthalene sulfonates via complexation by macrocyclic host cucurbit[7]uril)

RN 620161-23-1 HCAPLUS

CN 1-Naphthalenesulfonic acid, 8-(phenylamino)-, compd. with stereoisomer of tetradecahydro-2,18:3,17-dimethano-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,14a,15a,17,18,19a,20a,21a,22a,23a,24a,25a,26a,27a,28a,29a,30a-octacosazabispentaleno[1''',6''':5''',6''',7''']cycloocta[1''',2''',3''':3''',3''':3''',4''']pentaleno[1''',6''':5''',6''',7''']cycloocta[1'',2'',3'':3'',4'']pentaleno[1'',6'':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalenetetradecone (2:1) (9CI) (CA INDEX NAME)

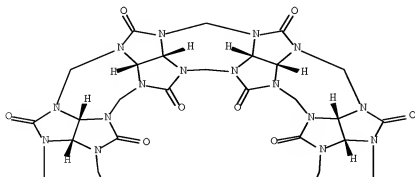
CM 1

CRN 259886-50-5

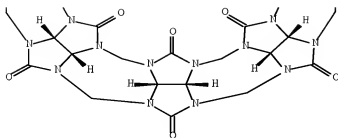
CMF C42 H42 N28 O14

Relative stereochemistry.

PAGE 1-A



PAGE 2-A



CM 2

CRN 82-76-8

CMF C16 H13 N O3 S



RN 620161-24-2 HCAPLUS

CN 2-Naphthalenesulfonic acid, 6-(phenylamino)-, compd. with stereoisomer of tetradecahydro-2,18:3,17-dimethano-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,14a,15a,17,18,19a,20a,21a,22a,23a,24a,25a,26a,27a,28a,29a,30a-octacosazabispentaleno[1''',6''':5''',6''',7''']cycloocta[1''',2''',3''':3''',4''']pentaleno[1''',6''':5''',6''',7''']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalenetetradecone (1:1) (9CI) (CA INDEX NAME)

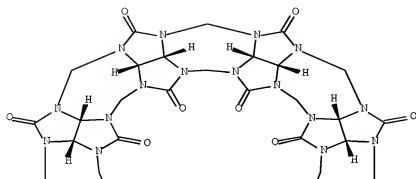
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CRN 259886-50-5

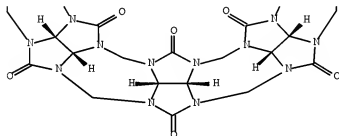
CMF C42 H42 N28 O14

Relative stereochemistry.

PAGE 1-A



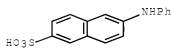
PAGE 2-A



CM 2

CRN 20096-53-1

CMF C16 H13 N O3 S



IT 259886-50-5, Cucurbit[7]uril

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent) (macrocyclic host; fluorescence enhancement of anilidonaphthalene sulfonates via complexation by macrocyclic host cucurbit[7]uril)

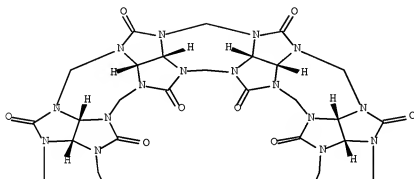
RN 259886-50-5 HCAPLUS

CN 2,18:3,17-Dimethano-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,14a,15a,17,18,19a,20a,21a,22a,23a,24a,25a,26a,27a,28a,29a,30a-octacosazabispentaleno[1''',6''':5'',6'',7''']cycloocta[1'',2'

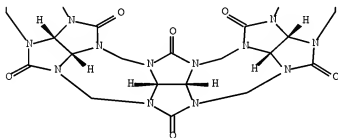
''',3''':3''',4''']pentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':
3'',4'']pentaleno[1'',6'':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
1,4,6,8,10,12,14,16,19,21,23,25,27,29-tetradecone, tetradecahydro-,
stereoisomer (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A



OSC.G 50 THERE ARE 50 CAPLUS RECORDS THAT CITE THIS RECORD (50 CITINGS)
RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 9 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN
AN 2003:590408 HCAPLUS Full-text
DN 139:135453
TI Cucurbiturils and method for binding gases and volatiles using
cucurbiturils
IN Day, Anthony Ivan; Arnold, Alan Peter; Blanch, Rodney John
PA Unisearch Limited, Australia
SO U.S. Pat. Appl. Publ., 12 pp., Cont.-in-part of U. S. Ser. No. 999,770.
CODEN: USXXCO
DT Patent
LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 20030140787	A1	20030731	US 2002-301874	20021122 <--
	US 6869466	B2	20050322		
	WO 2000068232	A1	20001116	WO 2000-AU412	20000505 <--
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	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 6793839	B1	20040921	US 2002-959770	20020107 <--
	AU 2002302117	A1	20030320	AU 2002-302117	20021122 <--
	AU 2002302117	B2	20060810		
	IN 2006DE02152	A	20070907	IN 2006-DE2152	20060928 <--
PRAI	US 1999-232	A	19990507	<--	
	WO 2000-AU412	W	20000505	<--	
	AU 2001-9031	A	20011122	<--	
	US 2002-959770	A2	20020107	<--	
	AU 2000-43851	A	20000505	<--	
	IN 2000-DE485	A3	20000508	<--	

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

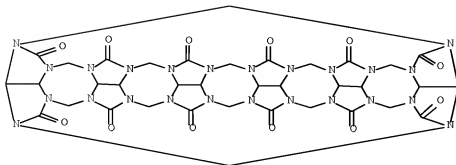
AB Gases or volatile compds. are bound by cucurbiturils as a cucurbituril-gas/volatile complex. The gases or volatile compds. can be separated from a mixture of compds. by contacting the mix with a cucurbituril whereby at least some of the gas or volatile compound is bound to the cucurbituril to form a cucurbituril complex, followed by the release of at least some of the bound gas or volatile compound from that complex. The use of cucurbiturils in binding gases and volatile compds. is suitable for storage, safety, delivery or other uses, such as the trapping of an unpleasant or toxic gas or volatile compound

IT 80262-44-8, Cucurbituril 143902-45-8,
Decamethylcucurbit [5]uril 259886-49-2, Cucurbit[5]uril
283175-97-3, Cucurbit [6]uril 569359-77-9
569363-90-2 569363-91-3

RL: TEM (Technical or engineered material use); USES (Uses)
(cucurbiturils and method for binding gases and volatiles using cucurbiturils)

RN 80262-44-8 HCAPLUS

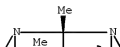
CN 1H, 4H, 14H, 17H-2, 16:3, 15-Dimethano-
5H, 6H, 7H, 8H, 9H, 10H, 11H, 12H, 13H, 18H, 19H, 20H, 21H, 22H, 23H, 24H, 25H, 26H-
2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 12a, 13a, 15, 16, 17a, 18a, 19a, 20a, 21a, 22a, 23a, 24
a, 25a, 26a-tetracosazabispentaleno[1'', 6'':5', 6'', 7'']cycloocta[1'', 2'',
3'':3', 4'']pentaleno[1'', 6'':5, 6, 7]cycloocta[1, 2, 3-gh:1', 2', 3'-
g'h']cycloocta[1, 2, 3-cd:5, 6, 7-c'd']dipentalene-
1, 4, 6, 8, 10, 12, 14, 17, 19, 21, 23, 25-dodecone, dodecahydro- (CA INDEX NAME)



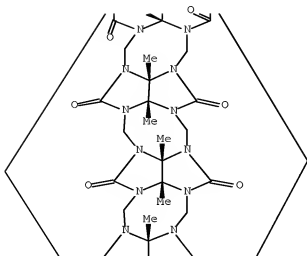
RN 143902-45-8 HCAPLUS
 CN 1H, 4H, 12H, 15H-2, 14:3, 13-Dimethano-
 5H, 6H, 7H, 8H, 9H, 10H, 11H, 16H, 17H, 18H, 19H, 20H, 21H, 22H-
 2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 13, 14, 15a, 16a, 17a, 18a, 19a, 20a, 21a, 22a-
 eicosazabispentaleno[1'', 6''':5'', 6'', 7'']cycloocta[1'', 2'', 3'':3', 4']pe
 ntaleno[1', 6':5, 6, 7]cycloocta[1, 2, 3-cd:1', 2', 3'-gh]pentalene-
 1, 4, 6, 8, 10, 12, 15, 17, 19, 21-decone, decahydro-
 2a, 13a, 15b, 16b, 17b, 18b, 19b, 20b, 21b, 22b-decamethyl-, stereoisomer (CA
 INDEX NAME)

Relative stereochemistry.

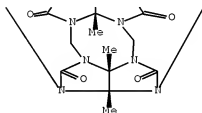
PAGE 1-A



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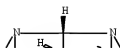
PAGE 3-A



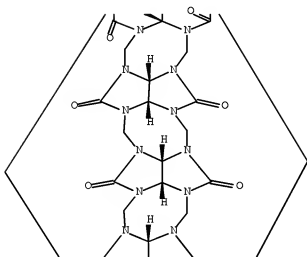
RN 259886-49-2 HCAPLUS
 CN 1H,4H,12H,15H-2,14:3,13-Dimethano-
 5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-
 2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-
 eicosazabispentaleno[1'',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pe
 ntaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
 1,4,6,8,10,12,15,17,19,21-decone, decahydro-, stereoisomer (CA INDEX
 NAME)

Relative stereochemistry.

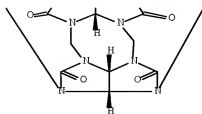
PAGE 1-A



PAGE 2-A



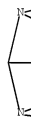
PAGE 3-A



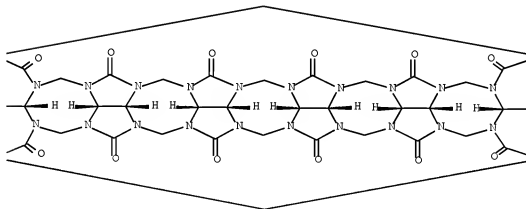
RN 283175-97-3 HCAPLUS
 CN 1H, 4H, 14H, 17H-2, 16:3, 15-Dimethano-
 5H, 6H, 7H, 8H, 9H, 10H, 11H, 12H, 13H, 18H, 19H, 20H, 21H, 22H, 23H, 24H, 25H, 26H-
 2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 12a, 13a, 15, 16, 17a, 18a, 19a, 20a, 21a, 22a, 23a, 24
 a, 25a, 26a-tetracosazabispentaleno[1'', 6'':5'', 6'':7'']cycloocta[1'', 2''
 , 3'':3', 4']pentaleno[1', 6':5, 6, 7]cycloocta[1, 2, 3-gh:1', 2', 3'-
 g'h']cycloocta[1, 2, 3-cd:5, 6, 7-c'd']dipentalene-
 1, 4, 6, 8, 10, 12, 14, 17, 19, 21, 23, 25-dodecone, dodecahydro-, stereoisomer (CA
 INDEX NAME)

Relative stereochemistry.

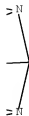
PAGE 1-A



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PAGE 1-C

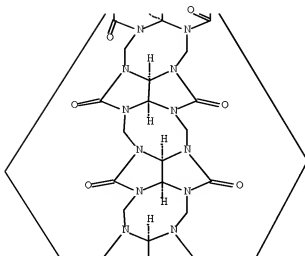


RN 569359-77-9 HCAPLUS
 CN 1H,4H,12H,15H-2,14:3,13-Dimethano-
 5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-
 2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-
 eicosazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pe
 ntaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
 1,4,6,8,10,12,15,17,19,21-decone, decahydro-2a,22b-dimethyl-, stereoisomer
 (CA INDEX NAME)

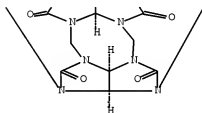
Relative stereochemistry.

PAGE 1-A





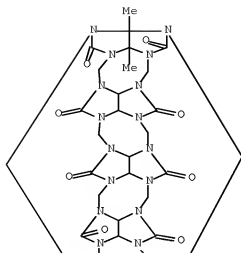
PAGE 2-A



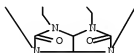
PAGE 3-A

RN 569363-90-2 HCAPLUS
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 5H, 6H, 7H, 8H, 9H, 10H, 11H, 16H, 17H, 18H, 19H, 20H, 21H, 22H-
 2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 13, 14, 15a, 16a, 17a, 18a, 19a, 20a, 21a, 22a-
 eicosazabispentaleno[1'', 6''':5'', 6'', 7'']cycloocta[1'', 2'', 3'':3', 4']pe
 ntaleno[1', 6':5, 6, 7]cycloocta[1, 2, 3-cd:1', 2', 3'-gh]pentalene-
 1, 4, 6, 8, 10, 12, 15, 17, 19, 21-decone, decahydro-2a, 13a, 15b, 22b(or
 2a, 17b, 17c, 22b)-tetramethyl-, stereoisomer (9CI) (CA INDEX NAME)

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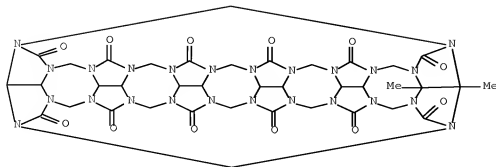


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2 (D1-Me)

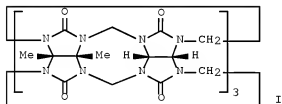
RN 569363-91-3 HCAPLUS
 CN 1H, 4H, 14H, 17H-2, 16:3, 15-Dimethano-
 5H, 6H, 7H, 8H, 9H, 10H, 11H, 12H, 13H, 18H, 19H, 20H, 21H, 22H, 23H, 24H, 25H, 26H-
 2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 12a, 13a, 15, 16, 17a, 18a, 19a, 20a, 21a, 22a, 23a, 24
 a, 25a, 26a-tetracosazabispentaleno[1'', 6'':5'', 6'':7'']cycloocta[1'', 2''
 , 3'':3', 4']pentaleno[1', 6':5, 6, 7]cycloocta[1, 2, 3-gh:1', 2', 3'-
 g'h']cycloocta[1, 2, 3-cd:5, 6, 7-c'd']dipentalene-
 1, 4, 6, 8, 10, 12, 14, 17, 19, 21, 23, 25-dodecone,
 dodecahydro-2a, 26b, ?, ?, ?-hexamethyl-, stereoisomer (9CI) (CA INDEX
 NAME)



4 (D1—Me)

OSC.G 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

L44 ANSWER 10 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN
 AN 2003:316145 HCAPLUS Full-text
 DN 140:77122
 TI A method for synthesizing partially substituted cucurbit[n]uril
 AU Day, Anthony I.; Arnold, Alan P.; Blanch, Rodney J.
 CS School of Chemistry, University College (UNSW), Australian Defence Force Academy, Canberra, ACT 2600, Australia
 SO Molecules (2003), 8(1), 74-84
 CODEN: MOLEFW; ISSN: 1420-3049
 URL: <http://www.mdpi.org/molecules/papers/80100074.pdf>
 PB Molecular Diversity Preservation International
 DT Journal; (online computer file)
 LA English
 OS CASREACT 140:77122
 GI



AB A novel approach to cucurbituril synthesis is described where partial substitution is introduced into cucurbit[n]uril. The identification of homologs (and their substitution) in reaction mixts. is achieved by a combination of ESMS and the use of the mol. probes (guests) 1,4-dioxane and 1,9-octanediamine. A unique sym. hexamethylcucurbit[3,3]uril (I), the major product, was isolated and characterized.
 IT 569359-17-9P 640732-36-1P 640732-37-2P
 640732-38-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (cyclocondensation of glycouril and its dimethyltetracyclic ether in preparation of partially substituted cucurbituril cyclic oligomers)
 RN 569359-77-9 HCAPLUS

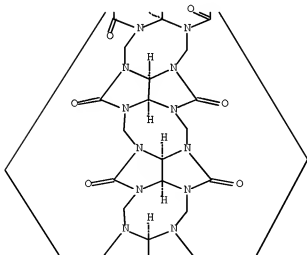
CN 1H, 4H, 12H, 15H-2, 14:3, 13-Dimethano-
 5H, 6H, 7H, 8H, 9H, 10H, 11H, 16H, 17H, 18H, 19H, 20H, 21H, 22H-
 2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 13, 14, 15a, 16a, 17a, 18a, 19a, 20a, 21a, 22a-
 eicosazabispentaleno[1''', 6''':5'', 6'', 7'']cycloocta[1'', 2'', 3'':3', 4']pe
 ntaleno[1', 6':5, 6, 7]cycloocta[1, 2, 3-cd:1', 2', 3'-gh]pentalene-
 1, 4, 6, 8, 10, 12, 15, 17, 19, 21-decone, decahydro-2a, 22b-dimethyl-, stereoisomer
 (CA INDEX NAME)

Relative stereochemistry.

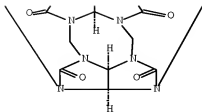
PAGE 1-A



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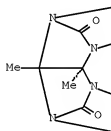
PAGE 3-A



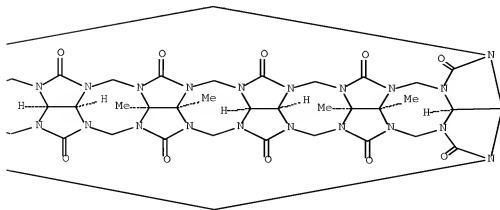
RN 640732-36-1 HCAPLUS
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 5H,6H,7H,8H,9H,10H,11H,12H,13H,18H,19H,20H,21H,22H,23H,24H,25H,26H-
 2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,15,16,17a,18a,19a,20a,21a,22a,23a,24
 a,25a,26a-tetracosazabispentaleno[1'',6'':5',6'',7'']cycloocta[1'',2''
 ,3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-
 g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
 1,4,6,8,10,12,14,17,19,21,23,25-dodecone,
 dodecahydro-2a,19b,19c,23b,23c,26b-hexamethyl-, stereoisomer (CA INDEX
 NAME)

Relative stereochemistry.

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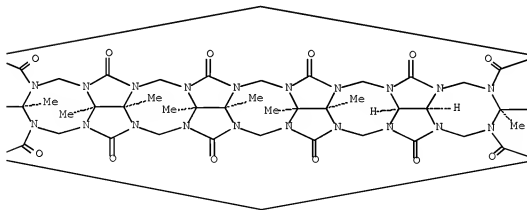
RN 640732-37-2 HCAPLUS
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 5H, 6H, 7H, 8H, 9H, 10H, 11H, 12H, 13H, 18H, 19H, 20H, 21H, 22H, 23H, 24H, 25H, 26H-
 2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 12a, 13a, 15, 16, 17a, 18a, 19a, 20a, 21a, 22a, 23a, 24
 a, 25a, 26a-tetracosazabispentaleno[1''', 6''' : 5'', 6'', 7'']cycloocta[1'', 2''
 , 3'' : 3', 4']pentaleno[1', 6' : 5, 6, 7]cycloocta[1, 2, 3-gh:1', 2', 3'-
 g'h']cycloocta[1, 2, 3-cd:5, 6, 7-c'd']dipentalene-
 1, 4, 6, 8, 10, 12, 14, 17, 19, 21, 23, 25-dodecone,
 dodecahydro-2a, 15a, 17b, 19b, 19c, 21b, 21c, 23b, 23c, 26b-decamethyl-,
 stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

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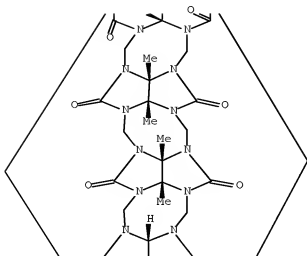
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 5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-
 2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-
 eicosazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pe
 ntaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
 1,4,6,8,10,12,15,17,19,21-decone, decahydro-2a,13a,15b,17b,17c,19b,19c,22b-
 octamethyl-, stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

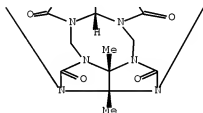
PAGE 1-A



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OSC.G 47 THERE ARE 47 CAPLUS RECORDS THAT CITE THIS RECORD (47 CITINGS)
 RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 11 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN

AN 2003:44731 HCAPLUS Full-text

DN 138:368812

TI The Effects of Alkali Metal Cations on Product Distributions in Cucurbit[n]uril Synthesis

AU Day, Anthony I.; Blanch, Rodney J.; Coe, Andrew; Arnold, Alan P.

CS University College (UNSW), School of Chemistry, Australian Defence Force Academy, Canberra, ACT 2600, Australia

SO Journal of Inclusion Phenomena and Macrocyclic Chemistry (2002), 43(3-4), 247-250

CODEN: JIICF5; ISSN: 1388-3127

PB Kluwer Academic Publishers

DT Journal

LA English

OS CASREACT 138:368812

AB Alkali metal cations act as templates in the synthesis of cucurbit[n]urils, Q[n], for n = 5-8, either from a preformed oligomer precursor, or directly from glycoluril and formaldehyde. Q[5] has been synthesized and isolated as an unusual, water-insol. potassium salt complex. The formation of this new

complex is a convenient method for isolating Q[5] as a salt from Q[n] mixts.

The complex is a convenient, high yielding source of Q[5].

IT 259886-45-2P, Cucurbit[5]uril 259886-50-5P,
Cucurbit[7]uril 259886-51-6P, Cucurbit[8]uril
283175-97-3P, Cucurbit[6]uril

RL: SPN (Synthetic preparation); PREP (Preparation)

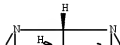
(effects of alkali metal cations on product distributions in
cucurbit[n]uril synthesis)

RN 259886-49-2 HCAPLUS

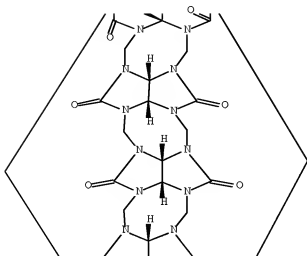
CN 1H, 4H, 12H, 15H-2, 14:3, 13-Dimethano-
5H, 6H, 7H, 8H, 9H, 10H, 11H, 16H, 17H, 18H, 19H, 20H, 21H, 22H-
2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 13, 14, 15a, 16a, 17a, 18a, 19a, 20a, 21a, 22a-
eicosazabispentaleno[1'', 6'':5'', 6'', 7'']cycloocta[1'', 2'', 3'':3', 4']pe
ntaleno[1', 6':5, 6, 7]cycloocta[1, 2, 3-cd:1', 2', 3'-gh]pentalene-
1, 4, 6, 8, 10, 12, 15, 17, 19, 21-decone, decahydro-, stereoisomer (CA INDEX
NAME)

Relative stereochemistry.

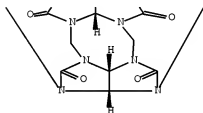
PAGE 1-A



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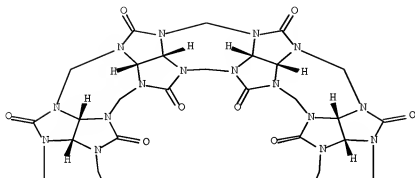
PAGE 3-A



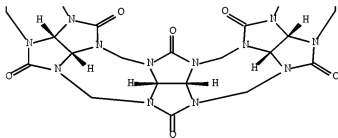
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 CN 2,18:3,17-Dimethano-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,14a,15a,17,18,19
 a,20a,21a,22a,23a,24a,25a,26a,27a,28a,29a,30a-
 octacosazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1''',2'
 ''',3''':3''',4''']pentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3''':
 3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
 1,4,6,8,10,12,14,16,19,21,23,25,27,29-tetradecone, tetradecahydro-,
 stereoisomer (CA INDEX NAME)

Relative stereochemistry.

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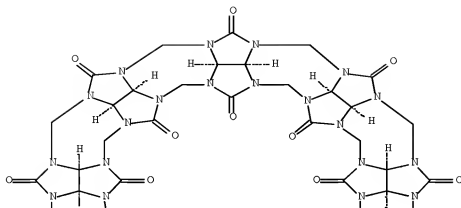
PAGE 2-A



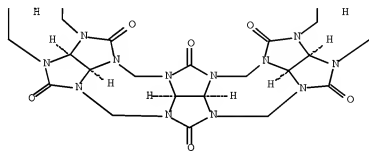
RN 259886-51-6 HCAPLUS
 CN 2,20:3,19-Dimethano-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,14a,15a,16a,17a,
 19,20,21a,22a,23a,24a,25a,26a,27a,28a,29a,30a,31a,32a,33a,34a-
 dotriacontaazabispentaleno[1''',6''':5''',6''',7''']cycloocta[1''',
 2''',3''':3''',4''']pentaleno[1'',6'':5'',6'',7'']cycloocta[1'',2'',3'
 '':3'',4'']pentaleno[1'',6'':5,6,7]cycloocta[1,2,3-gh:1',2',3'-
 g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
 1,4,6,8,10,12,14,16,18,21,23,25,27,29,31,33-hexadecone, hexadecahydro-,
 stereoisomer (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



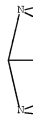
PAGE 2-A



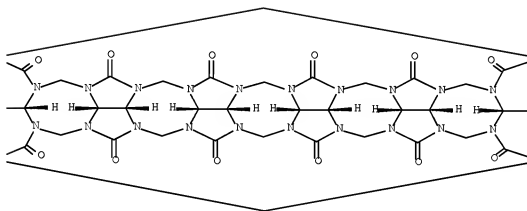
RN 283175-97-3 HCAPLUS
 CN 1H, 4H, 14H, 17H-2, 16:3, 15-Dimethano-
 5H, 6H, 7H, 8H, 9H, 10H, 11H, 12H, 13H, 18H, 19H, 20H, 21H, 22H, 23H, 24H, 25H, 26H-
 2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 12a, 13a, 15, 16, 17a, 18a, 19a, 20a, 21a, 22a, 23a, 24
 a, 25a, 26a-tetracosazabispentaleno[1'', 6'':5'', 6'', 7'']cycloocta[1'', 2''
 , 3'':3', 4']pentaleno[1', 6':5, 6, 7]cycloocta[1, 2, 3-gh:1', 2', 3'-
 g'h']cycloocta[1, 2, 3-cd:5, 6, 7-c'd']dipentalene-
 1, 4, 6, 8, 10, 12, 14, 17, 19, 21, 23, 25-dodecone, dodecahydro-, stereoisomer (CA
 INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 1-B



PAGE 1-C



OSC.G 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)
RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 12 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN

AN 2002:114457 HCAPLUS Full-text

DN 137:133907

TI The first endoannular metal halide-cucurbituril:

cis-SnCl₄(OH₂)₂@cucurbit[7]uril

AU Lorenzo, Susan; Day, Anthony; Craig, Don; Blanch, Rodney;

Arnold, Alan; Dance, Ian

CS School of Chemistry, University of New South Wales, Sydney, NSW 2052, Australia

SO CrystEngComm (2001) Paper No. 49, No pp. given, Paper No. 49

CODEN: CRECF4; ISSN: 1466-8033

URL: <http://www.rsc.org/CFCart/displayarticleonfree.cfm?article=A%2D9%223%24%5FV%3AB%214%2E%5FL9%28%3E%2CC%5B4MH1P%25H%3C%3E%5C6%2AQ%3E%3B1T%29XU%5BKG9%0A>

PB Royal Society of Chemistry

DT Journal; (online computer file)

LA English

AB The insertion and phys. entrapment of cis-SnCl₄(OH₂)₂ completely inside the annulus of the cyclic methylene-linked glycoluril heptamer known as cucurbit[7]uril (Q7) is described. This is the 1st endoannular metal halide-cucurbituril complex, [cis-SnCl₄(OH₂)₂]@Q7, contained in crystalline {[cis-SnCl₄(OH₂)₂]@Q7}·2.cntdot.(H₃O⁺)₆[SnCl₆]²⁻·3(H₂O)₂₃. The crystals are formed by reaction of Q7 and SnCl₄ in HCl. Crystals are orthorhombic, space group Fdd₂, with a 47.180(4), b 71.699(5), c 18.939(1) Å; Z = 16, dc = 1.76. The cis-SnCl₄(OH₂)₂ complex is contained completely within Q7, and is stabilized by the formation of excellent internal H bonds between coordinated H₂O and carbonyl O. The two crystallog. independent Q7 mols. in the crystal are incompletely occupied (75%, 50%), probably due to the premature crystallization of the insol. crystals. The crystal packing is analyzed in some detail to understand the low solubility and to enable formation of more soluble forms of [cis-SnCl₄(OH₂)₂]@Q7 which will allow development of its new coordination chemical. Some results of computational modeling of the dynamics of ingress of the chlorotin complexes into Q7 are reported.

IT 259886-50-5

RL: RCT (Reactant); RACT (Reactant or reagent)

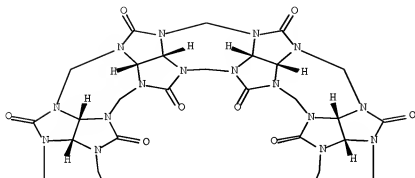
(for preparation of tin chloro aqua complex entrapped in cucurbituril)

RN 259886-50-5 HCAPLUS

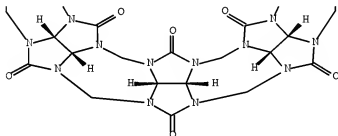
CN 2,18:3,17-Dimethano-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,14a,15a,17,18,19 a,20a,21a,22a,23a,24a,25a,26a,27a,28a,29a,30a-octacosazabispentaleno[1''',6''':5''',6''',7''']cycloocta[1''',2''':3''',3''':3''',4''']pentaleno[1''',6''':5''',6''',7''']cycloocta[1'',2'',3'':3'',4'']pentaleno[1'',6'':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentaleno-1,4,6,8,10,12,14,16,19,21,23,25,27,29-tetradecone, tetradecahydro-, stereoisomer (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



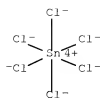
PAGE 2-A



IT 443927-25-2F
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation, crystal structure and DFT calcns. for formation of)
 RN 443927-26-2 HCAPLUS
 CN Tin, diaquatetrachloro-, (OC-6-22)-, compd. with dioxonium
 (OC-6-11)-hexachlorostannate(2-) and stereoisomer of
 tetradecahydro-2,18:3,17-dimethano-
 2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,14a,15a,17,18,19a,20a,21a,22a,23a,24
 a,25a,26a,27a,28a,29a,30a-
 octacosazabispentaleno[1''',6''':5''',6''',7''']cycloocta[1''',2'
 ''',3''':3''',4''']pentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':
 3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-
 gh]pentalenetetradecone (2:3:2), tricosahydrate (9CI) (CA INDEX NAME)

CM 1

CRN 443927-25-1
 CMF C16 Sn . 2 H3 O
 CCI CCS



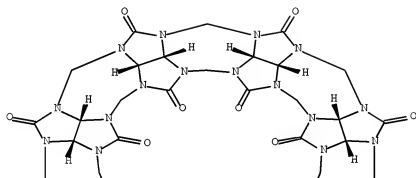
CM 2

CRN 259886-50-5

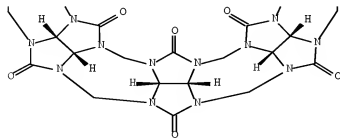
CMF C42 H42 N28 O14

Relative stereochemistry.

PAGE 1-A



PAGE 2-A

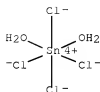


CM 3

CRN 37438-76-9

CMF C14 H4 O2 Sn

CCI CCS



RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 13 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN

AN 2002:108138 HCAPLUS [Full-text](#)

DN 136:401742

TI A cucurbituril-based gyroscane: a new supramolecular form

AU Day, Anthony I.; Blanch, Rodney J.; Arnold, Alan P.; Lorenzo,

Susan; Lewis, Gareth R.; Dance, Ian

CS School of Chemistry, University College, University of New South Wales

Australian Defence Force Academy, Canberra, 2600, Australia

SO Angewandte Chemie, International Edition (2002), 41(2), 275-277

CODEN: ACIEF5; ISSN: 1433-7851

PB Wiley-VCH Verlag GmbH

DT Journal

LA English

AB An inclusion complex of a cucurbit[5]uril with a cucurbit[10]uril is isolated in gram quantities and characterized by x-ray crystallog. In the crystal, a hydrate hydrochloride of the complex is isolated; a chloride ion (or hydrochloride salt) is sequestered within the cucurbit[5]uril ring, while the larger cucurbit[10]uril ring surrounds the cucurbit[5]uril ring but is not coaxial with it. The inclusion complex is termed a gyroscane because both cucurbituril rings rotate relative to one another in a manner similar to a gyroscope. Exchange expts. of the gyroscane with ¹³C-labeled-cucurbit[5]uril indicate that the cucurbit[5]uril ring exchanges slowly over time. No cucurbit[10]uril is isolated without included cucurbit[5]uril.

IT 430436-37-6

RL: PRP (Properties)

(crystal structure; preparation and X-ray crystallog. determination of a gyroscane inclusion complex of cucurbiturils)

RN 430436-37-6 HCAPLUS

CN 2,24:3,23-Dimethanotetracontaazabispentaleno[1''''''',6''''''':5''''''',6''
''',7''''''']cycloocta[1''''''',2''''''',3''''''':3''''''',4''''''']pentaleno[1''
''',6''''''':5''''''',6''''''',7''''''']cycloocta[1''''',2''''',3''''':3''''',4''''']pentaleno[1''',6''':5''',6''',7''']cycloocta[1'',2'',3'':3'',4'']pentaleno[1',6':5',6',7'
']cyclooct[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentaleneicosone, eicosahydro-, stereoisomer, compd. with stereoisomer of decahydro-1H,4H,12H,15H-2,14:3,13-dimethano-5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-eicosazabispentaleno[1''',6''':5''',6''',7''']cycloocta[1'',2'',3'':3'',4'']pentaleno[1',6':5',6',7']cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-1,4,6,8,10,12,15,17,19,21-decane, hydrochloride, hydrate (4:4:44:103)

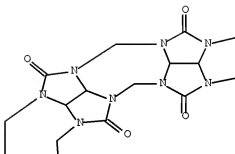
(9CI) (CA INDEX NAME)

CM 1

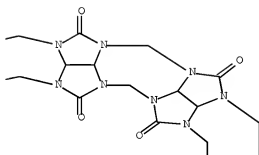
CRN 307001-50-9

CMF C60 H60 N40 O20

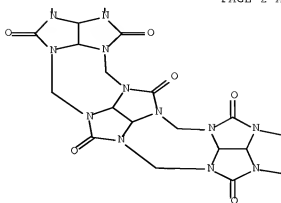
PAGE 1-A



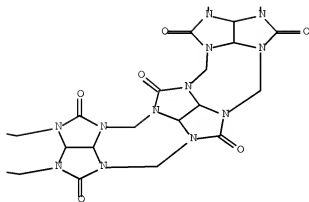
PAGE 1-B



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PAGE 2-B



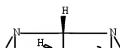
CM 2

CRN 259886-49-2

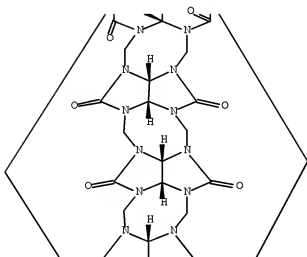
CMF C30 H30 N20 O10

Relative stereochemistry.

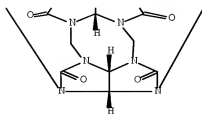
PAGE 1-A



PAGE 2-A



PAGE 3-A



IT 429697-51-8P

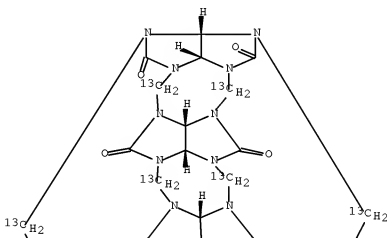
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process) (exchange of free cucurbiturils with a gyroscane inclusion complex of cucurbiturils)

RN 429697-51-8 HCAPLUS

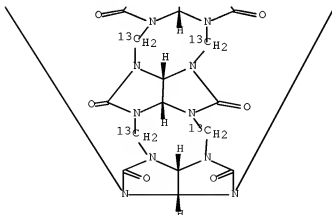
CN 1H, 4H, 12H, 15H-2, 14:3, 13-Dimethano-5H, 6H, 7H, 8H, 9H, 10H, 11H, 16H, 17H, 18H, 19H, 20H, 21H, 22H-2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 13, 14, 15a, 16a, 17a, 18a, 19a, 20a, 21a, 22a-eicosazabispentaleno[1'', 6''':5'', 6'', 7'']cycloocta[1'', 2'', 3'':3', 4']pentaleno[1', 6':5, 6, 7]cycloocta[1, 2, 3-cd:1', 2', 3'-gh]pentalene-1, 4, 6, 8, 10, 12, 15, 17, 19, 21-decone-5, 7, 9, 11, 16, 18, 20, 22, 23, 24-13C10, decahydro-, stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A



IT 430436-36-5P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(preparation and X-ray crystallog. determination of a gyroscane inclusion complex of cucurbiturils)

RN 430436-36-5 HCAPLUS

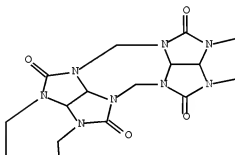
CN 2,24:3,23-Dimethanotetracontaazabispentaleno[1''''',6''''':5''''',6''''',7''''':5''''',6''''',7''''']cycloocta[1''''',2''''',3''''':3''''',4''''':3''''',4''''']pentaleno[1''''',6''''':5''''',6''''',7''''']cycloocta[1''''',2''''',3''''':3''''',4''''':3''''',4''''']pentaleno[1''''',6''''':5''''',6''''',7''''']cycloocta[1''''',2''''',3''''':3''''',4''''':3''''',4''''']pentaleno[1'',6':5,6,7]cyclooct[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentaleneicosone, eicosahydro-, stereoisomer, compd. with stereoisomer of decahydro-1H,4H,12H,15H-2,14:3,13-dimethano-5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-eicosazabispentaleno[1''''',6''''':5''''',6''''',7''''']cycloocta[1''''',2''''',3''''':3''''',4''''']pentaleno[1'',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-1,4,6,8,10,12,15,17,19,21-decone (1:1) (CA INDEX NAME)

CM 1

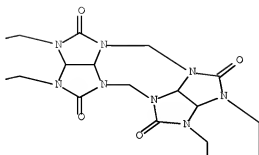
CRN 307001-50-9

CMF C60 H60 N40 O20

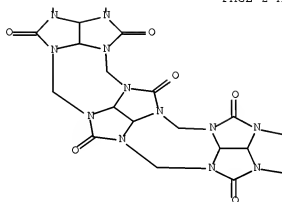
PAGE 1-A



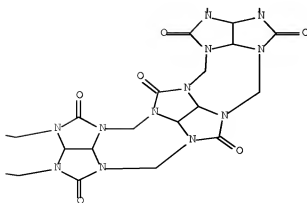
PAGE 1-B



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PAGE 2-B



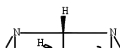
CM 2

CRN 259886-49-2

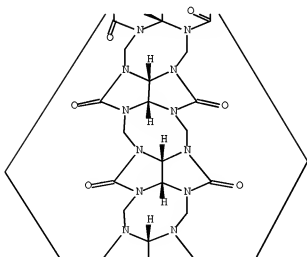
CMF C30 H30 N20 O10

Relative stereochemistry.

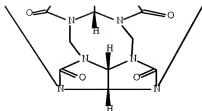
PAGE 1-A



PAGE 2-A



PAGE 3-A



OSC.G 135 THERE ARE 135 CAPLUS RECORDS THAT CITE THIS RECORD (136 CITINGS)
 RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 14 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN

AN 2001:878056 HCAPLUS Full-text

DN 136:151214

TI Cucurbit[7]uril and o-Carborane Self-Assemble to Form a Molecular Ball Bearing

AU Blanch, Rodney J.; Sleeman, Alex J.; White, Timothy J.; Arnold, Alan P.; Day, Anthony I.

CS School of Chemistry, University College, University of New South Wales, ADFA, Canberra, Australia

SO Nano Letters (2002), 2(2), 147-149

CODEN: NALEPD; ISSN: 1530-6984

PB American Chemical Society

DT Journal

LA English

OS CASREACT 136:151214

AB The self-assembly of cucurbit[7]uril (Q7) with o-carborane (1) produces a mol. ball bearing nanostructure. While investigating the possible role of o-carborane as a template for the controlled synthesis of Q7, new synthetic reaction conditions were discovered. Both the solvent and the reaction temperature had a marked effect on the relative percentages of cucurbit[n]uril (n = 5, 6, 7, 8) produced. The effect of the o-carborane in the reaction mixture is discussed.

IT 395660-22-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (inclusion complex; preparation and AM1 calcs. of)

RN 395660-22-7 HCAPLUS

CN 2,18:3,17-Dimethano-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,14a,15a,17,18,19 a,20a,21a,22a,23a,24a,25a,26a,27a,28a,29a,30a-octacosazabispentaleno[1''',6''':5''',6''',7''']cycloocta[1''',2''',3''':3''',4''']pentaleno[1''',6''':5''',6''',7''']cycloocta[1'',2'',3'':3'',4'']pentaleno[1'',6'':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalenetetradecone, tetradecahydro-, stereoisomer, compd. with 1,2-dicarbadodecaborane(12) (1:1) (9CI) (CA INDEX NAME)

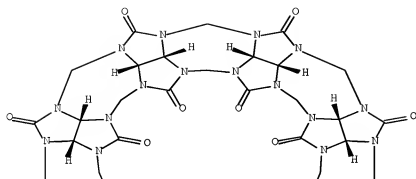
CM 1

CRN 259886-50-5

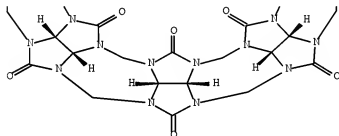
CMF C42 H42 N28 O14

Relative stereochemistry.

PAGE 1-A



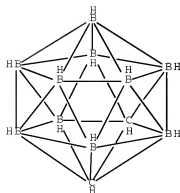
PAGE 2-A



CM 2

CRN 16872-09-6

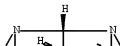
CMF C2 H12 B10



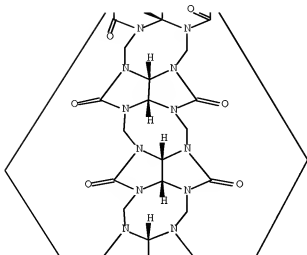
IT 259886-49-2P, Cucurbit[5]uril 259886-50-5P,
 Cucurbit[7]uril 259886-51-6P, Cucurbit[8]uril
 283175-97-3P, Cucurbit[6]uril
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 259886-49-2 HCAPLUS
 CN 1H, 4H, 12H, 15H-2, 14:3, 13-Dimethano-
 5H, 6H, 7H, 8H, 9H, 10H, 11H, 16H, 17H, 18H, 19H, 20H, 21H, 22H-
 2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 13, 14, 15a, 16a, 17a, 18a, 19a, 20a, 21a, 22a-
 eicosaazabispentaleno[1'', 6''':5'', 6'', 7'']cycloocta[1'', 2'', 3''':3', 4']pe
 ntaleno[1', 6':5, 6, 7]cycloocta[1, 2, 3-cd:1', 2', 3'-gh]pentalene-
 1, 4, 6, 8, 10, 12, 15, 17, 19, 21-decone, decahydro-, stereoisomer (CA INDEX
 NAME)

Relative stereochemistry.

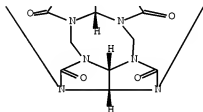
PAGE 1-A



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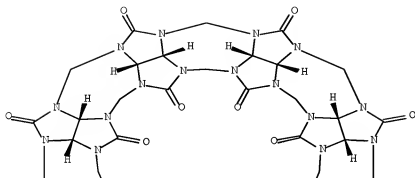
PAGE 3-A



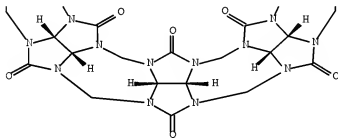
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 a,20a,21a,22a,23a,24a,25a,26a,27a,28a,29a,30a-
 octacosazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1''',2'
 ''',3''':3''',4''']pentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3''':
 3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
 1,4,6,8,10,12,14,16,19,21,23,25,27,29-tetradecone, tetradecahydro-,
 stereoisomer (CA INDEX NAME)

Relative stereochemistry.

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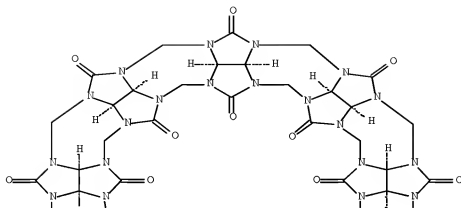
PAGE 2-A



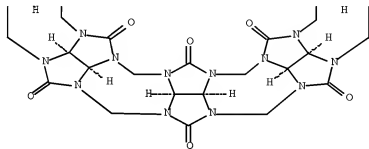
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 19,20,21a,22a,23a,24a,25a,26a,27a,28a,29a,30a,31a,32a,33a,34a-
 dotriacontaazabispentaleno[1''',6''':5''',6''',7''']cycloocta[1''',
 2''',3''':3''',4''']pentaleno[1'',6'':5'',6'',7'']cycloocta[1'',2'',3'
 '':3'',4'']pentaleno[1'',6'':5,6,7]cycloocta[1,2,3-gh:1',2',3'-
 g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
 1,4,6,8,10,12,14,16,18,21,23,25,27,29,31,33-hexadecone, hexadecahydro-,
 stereoisomer (CA INDEX NAME)

Relative stereochemistry.

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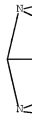
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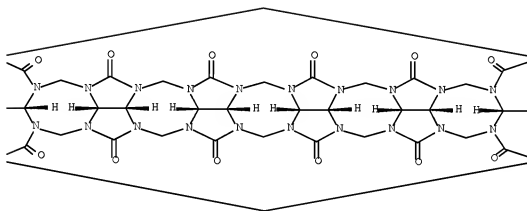
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 5H, 6H, 7H, 8H, 9H, 10H, 11H, 12H, 13H, 18H, 19H, 20H, 21H, 22H, 23H, 24H, 25H, 26H-
 2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 12a, 13a, 15, 16, 17a, 18a, 19a, 20a, 21a, 22a, 23a, 24
 a, 25a, 26a-tetracosazabispentaleno[1'', 6'':5'', 6'', 7'']cycloocta[1'', 2''
 , 3'':3', 4']pentaleno[1', 6':5, 6, 7]cycloocta[1, 2, 3-gh:1', 2', 3'-
 g'h']cycloocta[1, 2, 3-cd:5, 6, 7-c'd']dipentalene-
 1, 4, 6, 8, 10, 12, 14, 17, 19, 21, 23, 25-dodecone, dodecahydro-, stereoisomer (CA
 INDEX NAME)

Relative stereochemistry.

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OSC.G 54
RE.CNT 17

THERE ARE 54 CAPLUS RECORDS THAT CITE THIS RECORD (55 CITINGS)
THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 15 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN

AN 2001:809682 HCAPLUS Full-text

DN 136:85807

TI Controlling Factors in the Synthesis of Cucurbituril and Its Homologues

AU Day, Anthony; Arnold, Alan P.; Blanch, Rodney J.; Snushall, Barry

CS School of Chemistry University College, University of New South Wales, Australian Defence Force Academy, Canberra, 2600, Australia

SO Journal of Organic Chemistry (2001), 66(24), 8094-8100

CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

OS CASREACT 136:85807

AB The acid-catalyzed synthesis of cucurbit[n]urils from formaldehyde and glycoluril is poorly understood. A wide range of reaction conditions that include the effects of acid type, acid concentration, reactant concns., and temperature were examined to both probe the mechanism and optimize the yields of isolated cucurbit[n]urils [n = 5-10]. A mechanism for the formation of these cucurbit[n]urils is presented. Individual cucurbit[n]urils were unambiguously identified in reaction mixts. using ESMS and ¹³C NMR.

IT 143902-45-8 259886-49-2 259886-50-5

259886-51-6 283175-97-3 307001-50-9

375372-74-0 375372-75-1 375372-76-2

386768-89-4 386768-90-7 386768-91-8

386768-92-9 386768-93-0 386768-94-1

386768-95-2

RL: PRP (Properties)

(controlling factors in the synthesis of cucurbituril and its homologs)

RN 143902-45-8 HCAPLUS

CN 1H, 4H, 12H, 15H-2, 14:3, 13-Dimethano-

5H, 6H, 7H, 8H, 9H, 10H, 11H, 16H, 17H, 18H, 19H, 20H, 21H, 22H-

2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 13, 14, 15a, 16a, 17a, 18a, 19a, 20a, 21a, 22a-

eicosazabispentaleno[1'', 6''':5'', 6'', 7'']cycloocta[1'', 2'', 3''':3', 4']pe

ntaleno[1', 6':5, 6, 7]cycloocta[1, 2, 3-cd:1', 2', 3'-gh]pentalene-

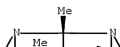
1, 4, 6, 8, 10, 12, 15, 17, 19, 21-decone, decahydro-

2a, 13a, 15b, 16b, 17b, 18b, 19b, 20b, 21b, 22b-decamethyl-, stereoisomer (CA

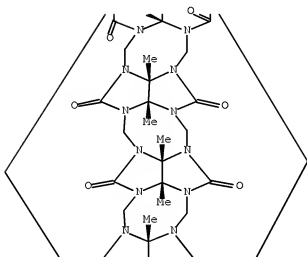
INDEX NAME)

Relative stereochemistry.

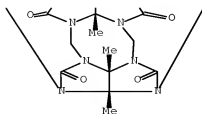
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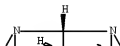
PAGE 3-A



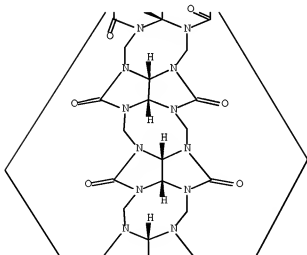
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 5H, 6H, 7H, 8H, 9H, 10H, 11H, 16H, 17H, 18H, 19H, 20H, 21H, 22H-
 2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 13, 14, 15a, 16a, 17a, 18a, 19a, 20a, 21a, 22a-
 eicosazabispentaleno[1''', 6''' : 5'', 6'', 7'']cycloocta[1'', 2'', 3'' : 3', 4']pe
 ntaleno[1', 6' : 5, 6, 7]cycloocta[1, 2, 3-cd: 1', 2', 3'-gh]pentalene-
 1, 4, 6, 8, 10, 12, 15, 17, 19, 21-decone, decahydro-, stereoisomer (CA INDEX
 NAME)

Relative stereochemistry.

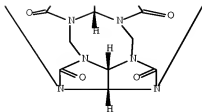
PAGE 1-A



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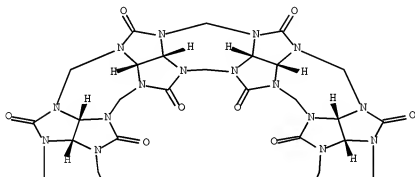


RN 259886-50-5 HCAPLUS

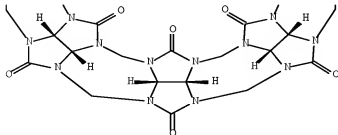
CN 2,18:3,17-Dimethano-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,14a,15a,17,18,19
 a,20a,21a,22a,23a,24a,25a,26a,27a,28a,29a,30a-
 octacosazabispentaleno[1''',6''':5''',6''',7''']cycloocta[1''',2''',3''':
 3'',4'']pentaleno[1'',6'':5'',6'',7'']cycloocta[1'',2'',3'':
 3',4']pentaleno[1,6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
 1,4,6,8,10,12,14,16,19,21,23,25,27,29-tetradecone, tetradecahydro-,
 stereoisomer (CA INDEX NAME)

Relative stereochemistry.

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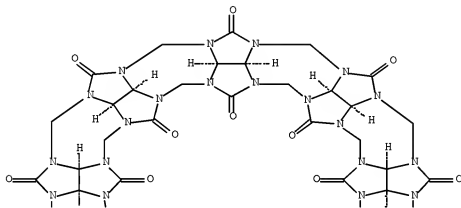
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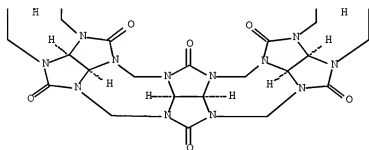
RN 259886-51-6 HCAPLUS
 CN 2,20:3,19-Dimethano-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,14a,15a,16a,17a,19,20,21a,22a,23a,24a,25a,26a,27a,28a,29a,30a,31a,32a,33a,34a-dotriacontaaazabispentaleno[1''',6''':5''',6''',7''']cycloocta[1''',2''',3''':3'',4'']pentaleno[1''',6''':5'',6''',7'']cycloocta[1'',2'',3''':3'',4'']pentaleno[1'',6'':5,6,7]cycloocta[1,2,3-gh:1'',2'',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-1,4,6,8,10,12,14,16,18,21,23,25,27,29,31,33-hexadecone, hexadecahydro-, stereoisomer (CA INDEX NAME)

Relative stereochemistry.

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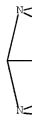
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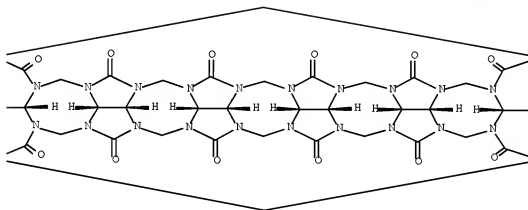
RN 283175-97-3 HCAPLUS
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Relative stereochemistry.

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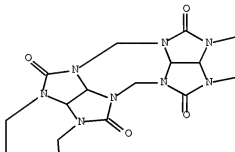


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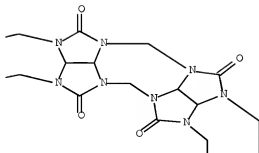


RN 307001-50-9 HCAPLUS
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 ''',7''''''']cycloocta[1''''',2''''',3''''':3''''',4''''']pentaleno[1''
 ''',6''''':5''''',6''''',7''''']cycloocta[1''''',2''''',3''''':3''''',4''''']pentale
 no[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3'',4'']pentaleno[1',6':5,6,7
]cyclooct[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-
 c'd']dipentaleneicosone, eicosahydro-, stereoisomer (CA INDEX NAME)

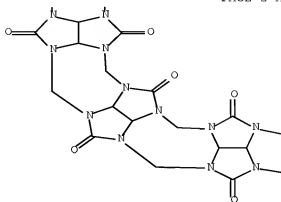
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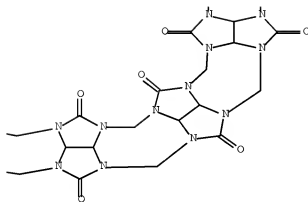
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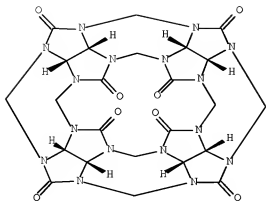
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RN 375372-74-0 HCAPLUS

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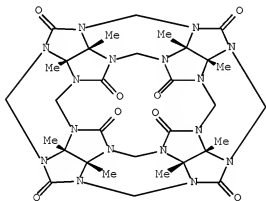
Relative stereochemistry.



RN 375372-75-1 HCAPLUS

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Relative stereochemistry.



RN 375372-76-2 HCAPLUS

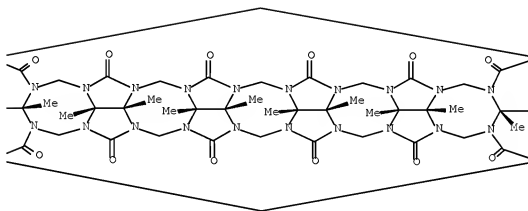
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Relative stereochemistry.

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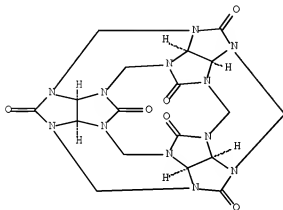
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RN 386768-89-4 HCAPLUS
 CN 1H, 4H, 8H, 11H-2, 10:3, 9-Dimethano-5H, 6H, 7H, 12H, 13H, 14H-
 2, 3, 4a, 5a, 6a, 7a, 9, 10, 11a, 12a, 13a, 14a-

dodecaazabispentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-1,4,6,8,11,13-hexone, hexahydro-, stereoisomer (9CI) (CA INDEX NAME)

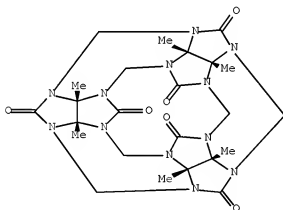
Relative stereochemistry.



RN 386768-90-7 HCAPLUS

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Relative stereochemistry.

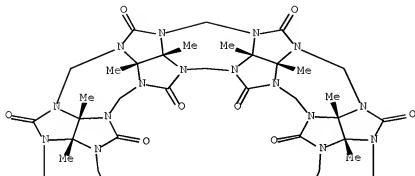


RN 386768-91-8 HCAPLUS

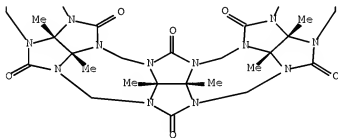
CN 2,18:3,17-Dimethano-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,14a,15a,17,18,19a,20a,21a,22a,23a,24a,25a,26a,27a,28a,29a,30a-octacosazabispentaleno[1''':6''':5''',6''',7''']cycloocta[1''',2''',3''':3''',4''']pentaleno[1''',6''':5''',6''',7''']cycloocta[1'',2'',3'':3'',4'']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalenetetradecone, tetradecahydro-2a,17a,19b,21b,21c,23b,23c,25b,25c,27b,27c,29b,29c,30b-tetradecamethyl-, stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

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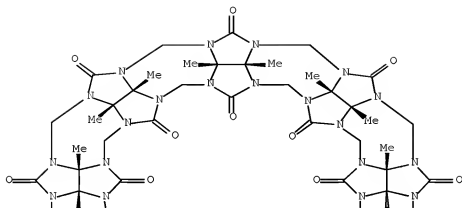
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RN 386768-92-9 HCAPLUS
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Relative stereochemistry.

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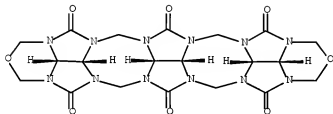


*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 386768-93-0 HCAPLUS

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(CA INDEX NAME)

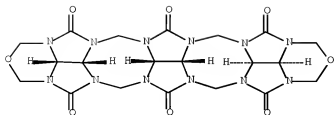
Relative stereochemistry.



RN 386768-94-1 HCAPLUS

CN 1H, 3H, 4H, 5H, 6H, 7H, 8H, 9H, 11H, 12H, 13H, 14H, 15H, 16H-2, 10-Dioxo-3a, 4a, 5a, 6a, 7a, 8a, 11a, 12a, 13a, 14a, 15a, 16a-dodecaazabisbenzo[3', 4']pentaleno[1', 6':5, 6, 7]cycloocta[1, 2, 3-cd:1', 2', 3'-gh]pentalene-4, 6, 8, 12, 14, 16-hexone, hexahydro-, (12ba, 12ca, 14ba, 14ca, 16bβ, 16cβ)- (9CI)
(CA INDEX NAME)

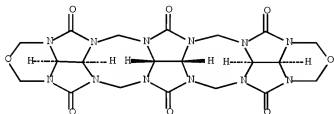
Relative stereochemistry.



RN 386768-95-2 HCAPLUS

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(CA INDEX NAME)

Relative stereochemistry.



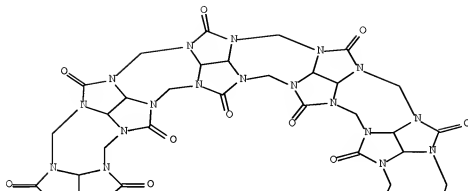
IT 387353-44-8P 387353-66-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(controlling factors in the synthesis of cucurbituril and its homologs)

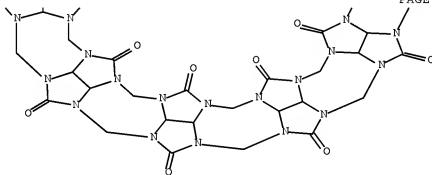
RN 387353-44-8 HCAPLUS

CN 1H, 4H, 20H, 23H-2, 22:3, 21-Dimethano-2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 12a, 13a, 14a, 15a, 16a, 17a, 18a, 19a, 21, 22, 23a, 24a, 25a, 26a, 27a, 28a, 29a, 30a, 31a, 32a, 33a, 34a, 35a, 36a, 37a, 38a-hexatriacontaazabispentaleno[1''''', 6''''':5''''', 6''''':7''''']cycloocta[1''''', 2''''':3''''':4''''']pentaleno[1''''', 6''''':5''''':6''''':7''''']cycloocta[1''''', 2''''':3''''':4''''']pentaleno[1''''', 6''''':5''''':6''''':7''''']cycloocta[1'', 2'', 3'':3'', 4'']pentaleno[1'', 6'':5, 6, 7]cycloocta[1, 2, 3-cd:1', 2', 3'-gh]pentaleneoctadecone, octadecahydro-, stereoisomer (CA INDEX NAME)

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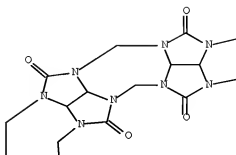
RN 387353-66-4 HCAPLUS
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 no[1''',6''':5'',6'',7''']cycloocta[1'',2'',3'':3',4']pentaleno[1'',6':5,6,7
]cyclooct[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-
 c'd']dipentaleneicosone, eicosahydro-, stereoisomer, compd. with
 stereoisomer of decahydro-1H,4H,12H,15H-2,14:3,13-dimethano-
 5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-
 2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-
 eicosazabispentaleno[1''',6''':5''',6'',7''']cycloocta[1''',2''',3'':3',4']pe
 ntaleno[1'',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
 1,4,6,8,10,12,15,17,19,21-decane (1:1), trihydrochloride (9CI) (CA INDEX
 NAME)

CM 1

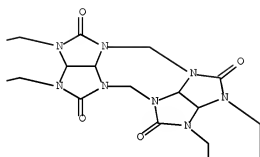
CRN 307001-50-9

CME C60 H60 N40 O20

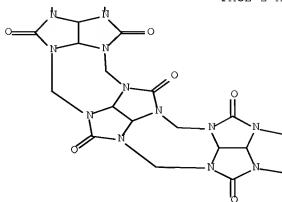
PAGE 1-A



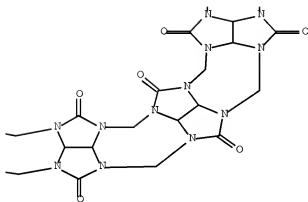
PAGE 1-B



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PAGE 2-B



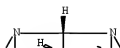
CM 2

CRN 259886-49-2

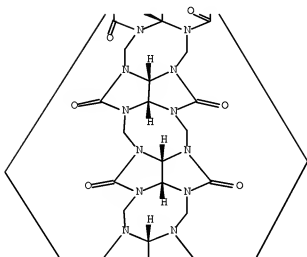
CMF C30 H30 N20 O10

Relative stereochemistry.

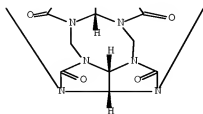
PAGE 1-A



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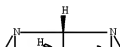
PAGE 3-A



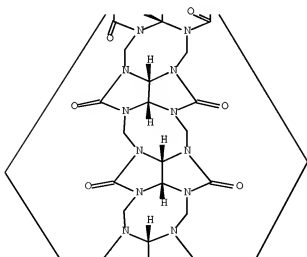
IT 386768-96-3P 386768-97-4P 386768-98-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (controlling factors in the synthesis of cucurbituril and its homologs)
 RN 386768-96-3 HCAPLUS
 CN 1H,4H,12H,15H-2,14:3,13-Dimethano-
 5H,6H,7H,8H,9H,10H,11H,16H,17H,18H,19H,20H,21H,22H-
 2,3,4a,5a,6a,7a,8a,9a,10a,11a,13,14,15a,16a,17a,18a,19a,20a,21a,22a-
 eicosazabispentaleno[1''',6''':5'',6'',7'']cycloocta[1'',2'',3'':3',4']pe
 ntaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
 1,4,6,8,10,12,15,17,19,21-decone, decahydro-, monohydrochloride,
 stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

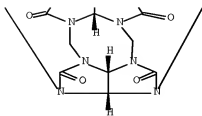
PAGE 1-A



PAGE 2-A



PAGE 3-A



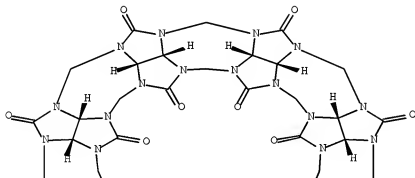
● HCl

RN 386768-97-4 HCAPLUS

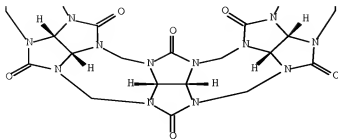
CN 2,18:3,17-Dimethano-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,14a,15a,17,18,19a,20a,21a,22a,23a,24a,25a,26a,27a,28a,29a,30a-octacosazabispentaleno[1''',6''':5''',6''',7''']cycloocta[1''',2''',3''',3''':4''']pentaleno[1''',6''':5''',6''',7''']cycloocta[1'',2'',3'':3',4']pentaleno[1',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalenetetradecone, tetradecahydro-, hydrochloride (2:1), stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

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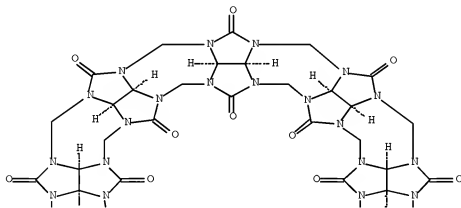
● 1/2 HCl

RN 386768-98-5 HCAPLUS

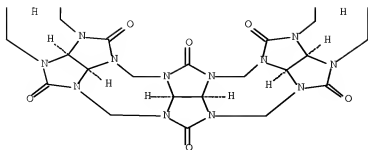
CN 2,20:3,19-Dimethano-2,3,4a,5a,6a,7a,8a,9a,10a,11a,12a,13a,14a,15a,16a,17a,19,20,21a,22a,23a,24a,25a,26a,27a,28a,29a,30a,31a,32a,33a,34a-dotriacontazabispentaleno[1''''',6''''':5''''',6''''',7''''']cycloocta[1''''',2''''',3''''':3''''',4''''']pentaleno[1''''',6''''':5''''',6''''',7''''']cycloocta[1'',2'',3''':3'',4'']pentaleno[1',6':5,6,7]cycloocta[1,2,3-gh:1',2',3'-g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalenehexadecone, hexadecahydro-, hydrochloride (2:5), stereoisomer (9CI) (CA INDEX NAME)

Relative stereochemistry.

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● 5/2 HCl

OSC.G 210 THERE ARE 210 CAPLUS RECORDS THAT CITE THIS RECORD (216 CITINGS)
 RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 16 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN

AN 2000:814488 HCAPLUS Full-text

DN 133:362775

TI Method for synthesis cucurbiturils

IN Day, Anthony Ivan; Arnold, Alan Peter

PA Unisearch Limited, Australia; Blanch, Rodney John

SO PCT Int. Appl., 112 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2000068232	A1	20001116	WO 2000-AU412	20000505 <--
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RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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EP 1181293	A1	20020227	EP 2000-924968	20000505 <--
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AU 777625	B2	20041021	AU 2000-43851	20000505 <--
CN 100339380	C	20070926	CN 2000-809064	20000505 <--
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KR 793461	B1	20080114	KR 2001-714227	20011107 <--
US 6793839	B1	20040921	US 2002-959770	20020107 <--
US 20030140787	A1	20030731	US 2002-301874	20021122 <--
US 6869466	B2	20050322		
IN 2006DE02152	A	20070907	IN 2006-DE2152	20060928 <--
FRAI AU 1999-232	A	19990507	<--	
WO 2000-AU412	W	20000505	<--	
IN 2000-DE485	A3	20000508	<--	
AU 2001-9031	A	20011122	<--	

US 2002-959770 A2 20020107 <--

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OS CASREACT 133:362775; MARPAT 133:362775

AB A method for producing cucurbit[n]urils, where n is from 4 to 12, comprising mixing substituted and/or unsubstituted glycoluril with an acid and a compound that can form methylene bridges between glycoluril units, and heating the mixture to a temperature of from 20° to 120° to thereby form cucurbit[n]. Novel cucurbit[n]urils, where n = 5, 6, 7, 8, 10 and substituted cucurbit[s,u]urils, where s = number of substituted glycoluril units, u = number of unsubstituted units and s + u = 4 - 12 are also described.

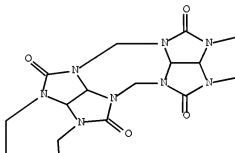
IT 307001-50-9P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and chemical shift of cucurbit[10]uril)

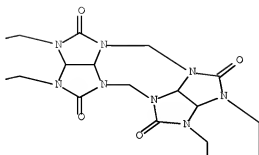
RN 307001-50-9 HCAPLUS

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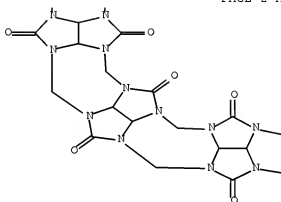
PAGE 1-A



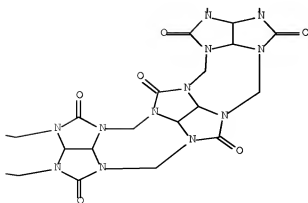
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IT 259886-45-2P 259886-50-5P 259886-51-6P
283175-97-3P

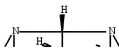
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of cucurbiturils)

RN 259886-49-2 HCAPLUS

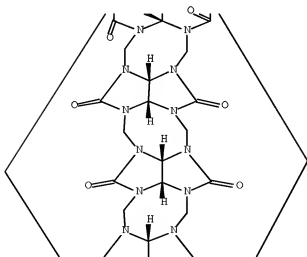
CN 1H, 4H, 12H, 15H-2, 14:3, 13-Dimethano-
5H, 6H, 7H, 8H, 9H, 10H, 11H, 16H, 17H, 18H, 19H, 20H, 21H, 22H-
2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 13, 14, 15a, 16a, 17a, 18a, 19a, 20a, 21a, 22a-
eicosazabispentaleno[1'', 6''':5'', 6'', 7'']cycloocta[1'', 2'', 3'':3', 4']pe
ntaleno[1', 6':5, 6, 7]cycloocta[1, 2, 3-cd:1', 2', 3'-gh]pentalene-
1, 4, 6, 8, 10, 12, 15, 17, 19, 21-decone, decahydro-, stereoisomer (CA INDEX
NAME)

Relative stereochemistry.

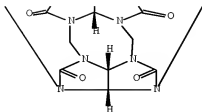
PAGE 1-A



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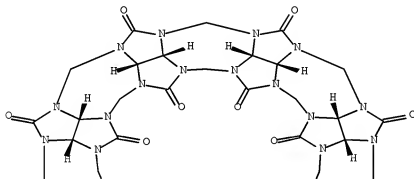
PAGE 3-A



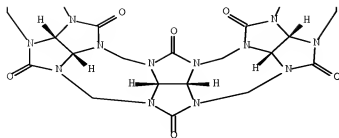
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 a,20a,21a,22a,23a,24a,25a,26a,27a,28a,29a,30a-
 octacosazabispentaleno[1''',6''':5''',6''',7''']cycloocta[1''',2'
 ''',3''':3''',4''']pentaleno[1''',6''':5''',6''',7''']cycloocta[1'',2'',3''':
 3'',4'']pentaleno[1'',6':5,6,7]cycloocta[1,2,3-cd:1',2',3'-gh]pentalene-
 1,4,6,8,10,12,14,16,19,21,23,25,27,29-tetradecone, tetradecahydro-,
 stereoisomer (CA INDEX NAME)

Relative stereochemistry.

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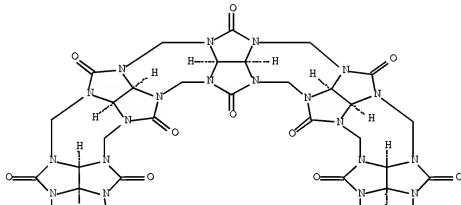
PAGE 2-A



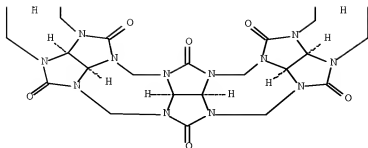
RN 259886-51-6 HCAPLUS
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 2''''',3''''':3''''',4''''']pentaleno[1''''',6''''':5''''',6''''',7''''']cycloocta[1'',2'',3
 ''':3'',4'']pentaleno[1'',6'':5,6,7]cycloocta[1,2,3-gh:1',2',3'-
 g'h']cycloocta[1,2,3-cd:5,6,7-c'd']dipentalene-
 1,4,6,8,10,12,14,16,18,21,23,25,27,29,31,33-hexadecone, hexadecahydro-,
 stereoisomer (CA INDEX NAME)

Relative stereochemistry.

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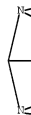
PAGE 2-A



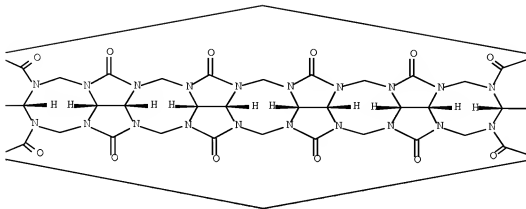
RN 283175-97-3 HCAPLUS
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 2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 12a, 13a, 15, 16, 17a, 18a, 19a, 20a, 21a, 22a, 23a, 24
 a, 25a, 26a-tetracosazabispentaleno[1'', 6'':5'', 6'', 7'']cycloocta[1'', 2''
 , 3'':3', 4']pentaleno[1', 6':5, 6, 7]cycloocta[1, 2, 3-gh:1', 2', 3'-
 g'h']cycloocta[1, 2, 3-cd:5, 6, 7-c'd']dipentalene-
 1, 4, 6, 8, 10, 12, 14, 17, 19, 21, 23, 25-dodecone, dodecahydro-, stereoisomer (CA
 INDEX NAME)

Relative stereochemistry.

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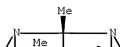
PAGE 1-C



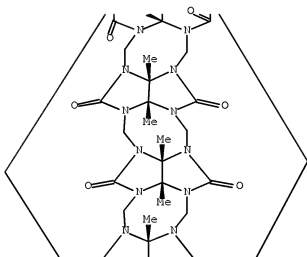
IT 143902-45-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of cucurbiturils)
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 5H, 6H, 7H, 8H, 9H, 10H, 11H, 16H, 17H, 18H, 19H, 20H, 21H, 22H-
 2, 3, 4a, 5a, 6a, 7a, 8a, 9a, 10a, 11a, 13, 14, 15a, 16a, 17a, 18a, 19a, 20a, 21a, 22a-
 eicosaazabispentaleno[1'', 6'':5'', 6'', 7'']cycloocta[1'', 2'', 3'':3', 4']pe
 ntaleno[1', 6':5, 6, 7]cycloocta[1, 2, 3-cd:1', 2', 3'-gh]pentalene-
 1, 4, 6, 8, 10, 12, 15, 17, 19, 21-decone, decahydro-
 2a, 13a, 15b, 16b, 17b, 18b, 19b, 20b, 21b, 22b-decamethyl-, stereoisomer (CA
 INDEX NAME)

Relative stereochemistry.

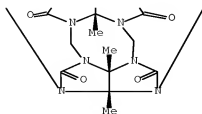
PAGE 1-A



PAGE 2-A



PAGE 3-A



OSC.G 40 THERE ARE 40 CAPLUS RECORDS THAT CITE THIS RECORD (40 CITINGS)
 RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> => d his

(FILE 'HOME' ENTERED AT 13:24:08 ON 02 DEC 2009)
 SET COST OFF

FILE 'HCAPLUS' ENTERED AT 13:24:32 ON 02 DEC 2009

L1 1 S US20070287836/PN OR (US2007-588846 OR WO2005-AU396 OR AU2004-
 E DAY
 E DAY/AU
 L2 150 S E3,E4
 E DAY ANTHONY/AU
 L3 39 S E3,E7,E8
 E DAY TONY/AU
 L4 696 S ?CUCURBITURIL?
 L5 25 S L1-L3 AND L4
 L6 1 S L1 AND L5
 L7 24 S L5 NOT L6
 SEL RN L6

FILE 'REGISTRY' ENTERED AT 13:27:06 ON 02 DEC 2009

L8 29 S E1-E29
 L9 1 S 80262-44-8
 L10 28 S L8 NOT L9

FILE 'HCAPLUS' ENTERED AT 13:28:35 ON 02 DEC 2009

L11 TRA L7 1- RN : 286 TERMS

FILE 'REGISTRY' ENTERED AT 13:28:36 ON 02 DEC 2009

L12 286 SEA L11
 L13 152 S L12 AND NR>=2 AND N>=4
 L14 STR
 L15 50 S L14
 L16 STR L14
 L17 50 S L16
 L18 5904 S L16 FUL
 SAV TEMP L18 NOBLE588A/A
 L19 28 S L8 AND L18
 L20 141 S L12 AND L18
 L21 148 S L19,L20

FILE 'HCAPLUS' ENTERED AT 13:33:34 ON 02 DEC 2009

L22 3123 S L18
 L23 25 S L22 AND L1-L3
 L24 1171 S L22 AND PY<=2005 NOT P/DT
 L25 1056 S L22 AND PY<=2004 NOT P/DT
 L26 2289 S L22 AND (PD<=20050318 OR PRD<=20050318 OR AD<=20050318)
 L27 2099 S L22 AND (PD<=20040319 OR PRD<=20040319 OR AD<=20040319)
 L28 17 S L24-L27 AND L23
 L29 2 S L24-L27 AND (A61K047-48 OR A61K0047-48)/IPC, IC, ICM, ICS, EPC

FILE 'REGISTRY' ENTERED AT 13:42:53 ON 02 DEC 2009

L30 STR L16
 L31 50 S L30 SAM SUB=L18
 L32 2546 S L30 FUL SUB=L18
 SAV TEMP L32 NOBLE588B/A

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FILE 'HCAPLUS' ENTERED AT 13:47:13 ON 02 DEC 2009
L33      806 S L32
L34      357 S L33 AND PY<=2005 NOT P/DT
L35      295 S L33 AND PY<=2004 NOT P/DT
L36      357 S L34,L35
L37      403 S L33 AND (PD<=20050318 OR PRD<=20050318 OR AD<=20050318)
L38      335 S L33 AND (PD<=20040319 OR PRD<=20040319 OR AD<=20040319)
L39      46 S L37,L38 NOT L36
          SEL HIT RN

FILE 'REGISTRY' ENTERED AT 13:48:52 ON 02 DEC 2009
L40      176 S E30-E205

FILE 'HCAPLUS' ENTERED AT 13:51:33 ON 02 DEC 2009
L41      24 S L1-L3 AND L33
L42      11 S L41 AND L36
L43      5 S L41 AND L39
L44      16 S L42,L43
L45      41 S L39 NOT L44

FILE 'REGISTRY' ENTERED AT 13:52:45 ON 02 DEC 2009

FILE 'HCAPLUS' ENTERED AT 13:52:56 ON 02 DEC 2009

FILE 'HCAPLUS' ENTERED AT 13:55:44 ON 02 DEC 2009
L46      346 S L36 NOT L44,L45
          SAV TEMP L46 NOBLE588C/A
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